4. DESIGN FRAMEWORK AND CONCEPTUALIZATION OF TRIM.Expo

The TRIM.Expo module is expected to estimate past and future human exposure patterns by combining pollutant concentration data with population activity tracking information. The estimation procedure requires (1) the use of algorithms to organize and manipulate pollutant concentration data and activity pattern information and (2) a process to define the link between the multimedia "ambient" environment and the microenvironmental exposure media that individuals occupy (*e.g.*, air compartments) or contact (*e.g.*, water, food, soil). Pollution concentration data are required as input into TRIM.Expo and can be derived from monitoring data, a single media transport model, or a multimedia transport model (*e.g.*, TRIM.FaTE).

The TRIM.Expo module provides a model framework addressing features unique to each problem and providing a characterization of the uncertainty associated with exposure estimates for single and multiple media pollutants. This includes a process for predicting concentrations in exposure media based on both the transfer from the ambient environment and on sources internal to those microenvironments containing the exposure media. This chapter describes the TRIM.Expo modeling system and how it was conceptualized to meet the above goals.

In order to characterize aggregate human exposure to a pollutant, each exposure route and pathway must be considered. For example, a semi-volatile hazardous air pollutant (*e.g.*, aromatic hydrocarbon) that is released to ambient air can be transported to multiple locations where exposure may occur. The pollutant can be (1) transported to the indoor or outdoor air surrounding a human receptor who would then inhale the pollutant; (2) transferred by deposition and run-off to surface water that supports fish consumed by the human receptor or provides drinking water to the human receptor; or (3) transferred by deposition to vegetation that is consumed by the human receptor or to vegetation that is consumed by the animals that supply meat and milk that is consumed by the human receptor. Each scenario defines a pathway from the pollutant's air emission to a receptor's contact with it via an associated route of contact. Total exposure cannot be estimated until the pathways and routes that account for a substantial amount of the intake and uptake for a receptor population have been identified.

The TRIM.Expo module is designed to be used by analysts (*e.g.*, modelers) and decision-makers (*e.g.*, regulators). As part of the initial development of TRIM. Expo, questions and issues regarding pollutant exposure of concern to analysts and decision-makers were identified.

Some of the more significant questions pertinent to analysts include the following.

- Which input properties are the most critical for modeling the movement and persistence of chemicals in indoor and outdoor environments, and which are of lesser importance, for estimating human exposures?

- How reliable are the ambient and/or microenvironmental concentration data used as input to the model, and how does the reliability of these concentrations limit the reliability of the exposure estimate?

Some of the more significant questions pertinent to decision-makers include the following.

- For a given pollutant emission control measure or magnitude of reduction in ambient pollutant levels, how much reduction of exposure (and related health effects) can be expected?

- What is an indicator of exposure that can be estimated? How much of a change can be estimated in this indicator to provide evidence that a control measure might be effective?

- How long is the lag time between a change in pollutant emissions and the estimated change in the environment or exposure indicator?

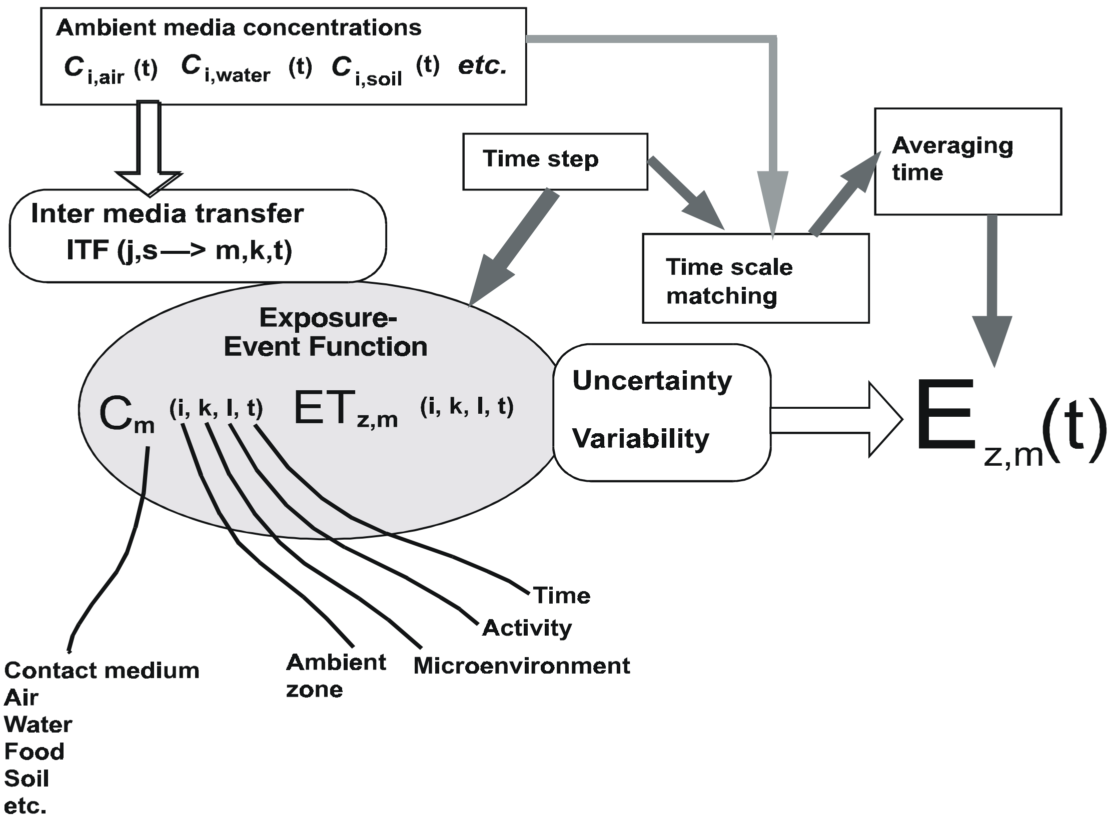
- How likely are these estimates to be wrong? How uncertain are the quantitative estimates of exposure reduction and changes in environmental indicators of exposure?

To answer the questions identified above, a taxonomy of exposure questions was formulated (see Section 2.3). From this, a prioritized set of exposure-model attributes was selected, resulting in three primary model dimensions.

4.1 EXPOSURE-EVENT MODULE STRUCTURE

Exposure events are activities that bring people in contact with a contaminated exposure medium in a specified microenvironment within a given exposure district. To construct exposure events, an individual or a cohort must be linked with a series of time-specific activities and with the exposure districts and microenvironments associated with those activities. In addition, pollutant concentrations in each district-microenvironment combination must be defined through a combination of databases and stochastic process models. This process of constructing exposure events is illustrated in Figure 4-1. Exposure-event simulations must be able to provide a broad range of information, including (1) detailed information on the input distributions selected (*e.g.*, relative probability of values, fractiles and central tendency, confidence intervals, shape of the distribution); (2) detailed information on the output distribution (the information here would follow in a similar fashion to item 1, above); (3) information about the goodness-of-fit of the data; (4) information about interdependencies and correlations between variables; (5) the number of times the concentration exceeded specified concentration levels; (6) the average exposure concentration exceeding some specified level; and (7) the cumulative intake or uptake during a series of exposure events. The TRIM.Expo module will contain algorithms that determine all of these parameters. These algorithms will include the basic exposure-event function, the average exposure concentration, the intake-adjusted average exposure concentration, the intermedia transfer factor, and the average daily potential dose.

Figure 4-1
Illustration of an Exposure-Event Simulation



4.1.1 BASIC EXPOSURE-EVENT FUNCTION

The basic exposure-event function determines the microenvironmental exposure to an individual or cohort from an exposure medium during time step, *t*. It defines exposure as the product of concentration and exposure duration, as illustrated in Figure 4-1 and shown in Equation 4-1. This equation can also be used to define an exposure concentration in other media, such as water and food, although it is less intuitive than an exposure of mg/kg-body-weight for food. For exposure media such as food and water, the potential dose rate is preferred as a basis for intake estimates (see Section 4.1.5).

$$E_{z,m}(t) = C_m(i,k,l,t)ET_{z,m}(i,k,l,t) \tag{4-1}$$

where

$E_{z,m}$ = Exposure experienced by person *z* from exposure medium *m* during time step t, given that person *z* is in exposure district *i* in microenvironment *k* conducting activity *l* during that time step *t*. For example, the exposure in air might be measured in units of mg-hr/m^3. Note that the exposure time need not be a whole time step.

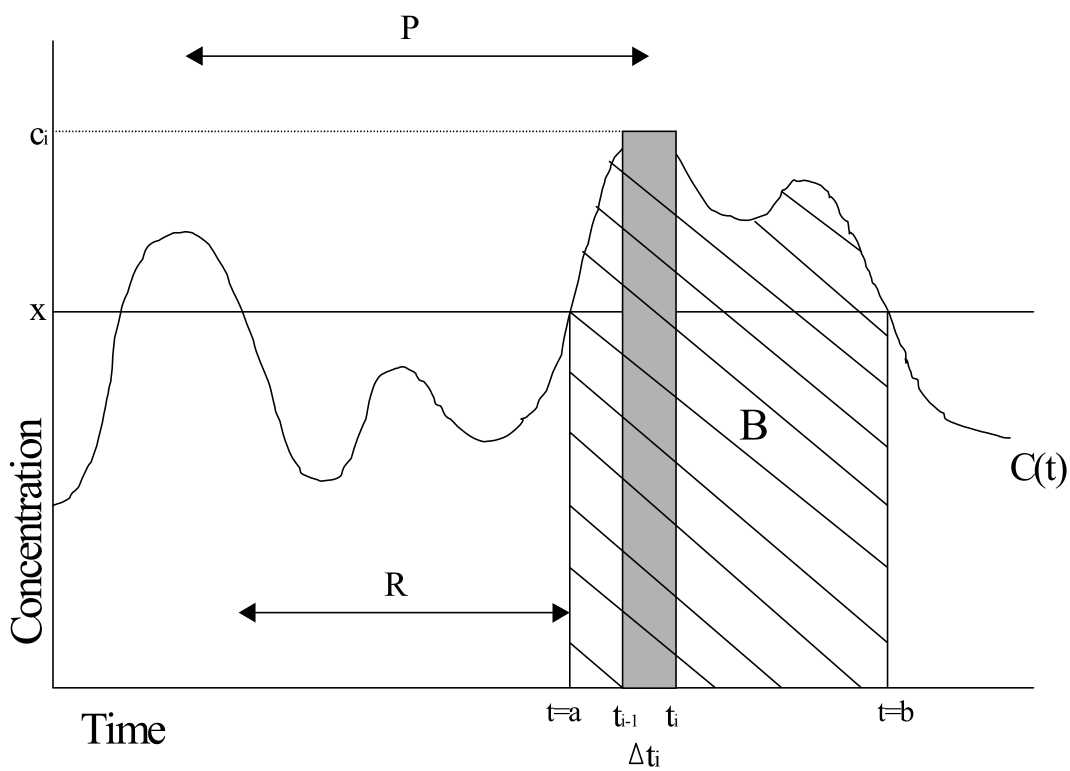
C_m	=	Concentration in exposure medium *m* (*e.g.*, air, water, soil) in exposure district *i* in microenvironment *k* associated with activity *l* during time step *t*. Units of measurement for air might be mg/m^3, while units of measurement of food might be mg/kg.
$ET_{z,m}$	=	Exposure duration of individual or cohort *z* to exposure medium *m* in exposure district *i* in microenvironment *k* conducting activity *l* during time step *t*.
z	=	Individual or cohort.
m	=	Exposure medium contacted (*i.e.*, air, water, food).
i	=	Exposure district.
k	=	Microenvironment in which the exposure occurs (*e.g.*, indoors at home, in a vehicle, indoors at work).
l	=	Activity code that describes what the individual is doing at the time of exposure (*e.g.*, resting, working, preparing food, cleaning, eating).

4.1.2 EXPOSURE OR POTENTIAL DOSE PROFILES

The time series of concentrations that could potentially result in an exposure comprises a profile, as illustrated in Figure 4-2. As shown in Equation 4-1, exposure to a pollutant is calculated as the product of the concentration that a person contacts and the duration of the contact. This is shown graphically in Figure 4-2. The x-axis shows the time sequence, while the y-axis shows the concentration of a pollutant. Therefore, the concentration for each instant in time is given by the curve, *C(t)*. To simplify the discussion, suppose that a person was in a particular microenvironment from time t_{i-1} to t_i and that the concentration of the pollutant (given by c_i) remained fairly constant during this time period (to make this example as simple as possible $t_i - t_{i-1} = \Delta t_i$ is defined as one hour). The shaded rectangle in Figure 4-2 has height c_i and width Δt_i. The area given by this rectangle is, therefore, c_i (Δt_i) and as stated above and shown in Equation 4-1 the product of a concentration and a time interval is equal to exposure. Thus, the area given by the shaded rectangle approximates the person's exposure over the time interval from t_{i-1} to t_i. The sum of the areas of many such rectangles from time *a* to time *b* approximates the person's exposure for this interval of time and applies whether the person remains in a single microenvironment or visits many microenvironments. Therefore, the hatched area given by *B* in Figure 4-2 is the person's integrated exposure from time *a* to time *b*.

If a dose metric, such as breathing rate or ingestion rate, had been included with the information on concentration, then the profile in Figure 4-2 would approximate the potential dose. The dose profile combines information on pollutant concentrations, activity patterns, and intake rates. For many pollutants (*e.g.*, ozone, carbon monoxide), the time series of exposure or potential dose may be more important for estimating the health impact than the overall average exposure or cumulative dose (McCurdy 1997). Figure 4-2 also shows some of the measures of exposure or potential dose that may be derived from the profile. The output options for TRIM.Expo will include exposure and potential dose profiles.

Figure 4-2
Example of an Exposure or a Potential Dose Profile and Associated Measures (adapted from McCurdy 1997)



KEY

B	=	integrated exposure from time *t=a* to *t=b*
P	=	time between peaks over *x*
R	=	respites between exceedances of *x*

The method of combining the vital information that is used in a dose profile makes it possible to develop estimates for alternative exposure and dose metrics for different averaging times from one hour to a year or more. Examples of alternative metrics that OAQPS has needed to investigate recently include children exposed to 8-hour daily ozone values greater than 0.08 ppm while exercising at a breathing rate of 15 L/min/m^2 or higher, and cardiovascular-impaired persons with a daily carboxyhemoglobin level of 2 percent or higher due to CO exposures (McCurdy 1995). Indeed, by using this disaggregated approach, almost any combination of exposure and dose metrics is possible.

With respect to health effects, two important considerations are (1) the time-scale of the health effects that result from an exposure or repeated exposures and (2) whether there is assumed to be a threshold concentration below which no health impacts are expected. Depending upon the health effects associated with the pollutant of interest, the exposure and potential dose profile may be used to derive several metrics. For example, if the time steps are one-hour, each concentration estimate represents a one-hour average. If the pollutant's health effect is associated with one-hour average exposures and has a lowest observed or a no observed adverse effect level (*e.g.*, x), important metrics might include the following (refer to Figure 4-2).

1. The number of person-hours of exposure to concentrations above x:

$$= P(cohort) \times \sum_t [\partial(t) \times C(t)] \qquad (4\text{-}2)$$

where:

$P(cohort)$	=	population of the cohort,
$\partial(t)$	=	0 if $C(t) \leq x$, 1 if $C(t) > x$, and
$C(t)$	=	exposure concentration for time step t.

2. The sum of the concentrations that exceed x

$$= \sum_t [\partial(t) \times C(t)] \qquad (4\text{-}3)$$

where:

t = $a, t_1, t_2, \ldots, t_{n-1}, t_n = b$ (refer to Figure 4-2).

3. The average of the concentrations that exceed x

$$= \frac{\sum_t [\partial(t) \times C(t)]}{\sum_t \partial(t)} \qquad (4\text{-}4)$$

4. The sum of exceedances of x, when it is exceeded

$$= \sum_t [\partial(t) \times \{C(t) - x\}] \qquad (4\text{-}5)$$

where:

t = $a, t_1, t_2, \ldots, t_{n-1}, t_n = b$ (refer to Figure 4-2).

5. The average exceedance of *x*, when it is exceeded

$$= \frac{\sum_t [\partial(t) \times \{C(t) - x\}]}{\sum_t \partial(t)} \qquad (4\text{-}6)$$

Other important metrics might include the average number of sequential hours exceeding *x*, or the average number of time steps between local concentration peaks (*i.e.*, average length of respites).

If the pollutant's health effect does not have a specific benchmark concentration (*i.e.*, lowest observed or no observed adverse effect level), but is associated with a certain averaging time (*e.g.*, 1-hour, 8-hour, 24-hour, annual), important metrics might include:

- The distribution of the maximum concentration corresponding to the averaging time of interest for the exposure period, typically one year (*e.g.*, distribution of the maximum 8-hour average concentration for any time during the year), or
- The average daily maximum concentration corresponding to the averaging time of interest for the exposure period (*e.g.*, the average of the maximum 8-hour average concentration for each day of the year).

The TRIM.Expo module was designed to address OAQPS' need for an integrated exposure model system that can evaluate the distribution of the population exposed to specified levels of air pollution and the number of times they are exposed for one-hour, eight-hour, monthly, quarterly, seasonal, and annual averaging periods (McCurdy 1995). As described above, TRIM.Expo will fulfill this need by producing population distributions of multiple exposure, dose, and dose-rate indicators.

4.1.3 AVERAGE EXPOSURE CONCENTRATION

During a relatively long time period (*e.g.*, day, week, year), individuals have different time/activity budgets and occupy different microenvironments with different pollutant concentrations. In such cases, exposure cannot be addressed by using the basic exposure-event function. Duan (1982) proposed a method to determine the average exposure concentration, $EC_{z,m}$, that has been used by others (Ott 1984, Ott et al. 1988, Ott et al. 1992a, Klepeis 1994, Lurmann and Korc 1994, MacIntosh et al. 1995):

$$EC_{z,m} = \frac{1}{T} \sum_t C_m(i,k,l,t) ET_{z,m}(i,k,l,t) \qquad (4\text{-}7)$$

where:

$EC_{z,m}$ = average exposure concentration in exposure medium *m* of individual or cohort *z* over time period *T*, where *T* is used as the averaging time and is the sum of all time steps, *t*

T = sum of all time steps, *t*.

The algorithm would determine an exposure concentration averaged over the total potential exposure duration considered in a specific TRIM.Expo application. However, the averaging time may not correspond to the averaging time specified for a health benchmark. For example, the exposure averaging time for a particular application of TRIM.Expo may be a year, while the averaging time for the health benchmark for the pollutant may be specified for a lifetime. Such issues will need to be addressed in TRIM's Risk Characterization module, TRIM.Risk.

4.1.4 INTAKE-ADJUSTED AVERAGE EXPOSURE CONCENTRATION

Cumulative exposure can also be determined using overall average concentration of the exposure medium that enters the body over time period *T*. The intake-adjusted average exposure concentration, IEC_z, is calculated using a weighting factor based on the intake rate, such as breathing or ingestion rate:

$$IEC_z = \frac{\sum_t C_m(i,k,l,t)ET_z(i,k,l,t)IU_{m,z}(t)}{\sum_t ET_z(i,k,l,t)IU_{mz}(t)} \qquad (4\text{-}8)$$

where

$IU_{m,,z}(t)$ = rate of intake/uptake in exposure medium *m* by individual or cohort *z* during an exposure time step *t*, and under other factors that are defined above. For food ingestion, the units of measurement for IU_{mz} might be kg-food/kg-body-weight during an exposure duration *ET*.

4.1.5 INTERMEDIA TRANSFER FACTOR

In many situations, the concentration in the exposure medium, C_m, is not known directly and must be estimated from an intermedia transfer. For example, the outdoor air concentration of a particular pollutant may be known, but the pollutant concentration indoors and the exposure medium may be unknown. To differentiate the indoor air concentration contribution from that of the outdoor air requires an intermedia transfer factor, which converts the time history of concentrations that is known (*i.e.*, outdoor air) to an estimate of the time history of the unknown concentration (*i.e.*, indoor air). Other examples of intermedia transfers include soil to house dust, water to indoor air, water to fish, and soil to home-grown vegetables.

The intermedia transfer factor, *ITF*, is used as follows:

$$C_m(i,k,l,t) = \sum_j \sum_s C_n(j,s) ITF(j,s \Rightarrow m,k,t) \qquad (4\text{-}9)$$

In this expression, for exposure medium *m* (*e.g.*, air, water, soil) at location *i* in microenvironment *k* associated with activity *l* during time step *t*, $C_m(i,k,l,t)$ is the concentration contributed by concentration $C_n(j,s)$ from environmental medium *n* at location *j* and time *s*. $ITF(j,s \rightarrow m,k,t)$ is the intermedia transfer algorithm that maps concentration $C_n(j,s)$ to concentration $C_m(i,k,l,t)$. Summation of the product $C_n \times ITF$ time occurs over previous time steps that impact current time step *t* and over all locations *j* that impact current microenvironment *k*.

4.1.6 AVERAGE DAILY POTENTIAL DOSE

The exposure-event function is frequently used to assess the potential dose to an exposed individual from his or her cumulative intake over some time period relative to an averaging time. The average daily potential dose, ADD_{pot}, is the potential dose per day (d). It is similar to the intake-adjusted average exposure concentration, but defines an average rate of intake in mg/kg/d or mg/d over the averaging time instead of a concentration.

$$ADD_{pot} = \frac{\sum \left(C_m(i,k,l,t) ET_{z,m}(i,k,l,t) IU_{z,m}(t) \right)}{T} \qquad (4\text{-}10)$$

where:

T	=	averaging time used to assess the health effects of the intake,
$IU_{z,m}(t)$	=	rate of intake/uptake.

4.2 DEFINING THE MODEL COMPONENTS FOR A TRIM.Expo APPLICATION

To set up a TRIM.Expo application, several steps must be performed.

1. Identify the pollutant(s) of interest, the study area, the exposure districts, and the population(s) of interest.

2. Determine environmental media within each exposure district. Estimate ambient media and time-varying pollutant concentrations in the environmental media.

3. Identify exposure media for the population(s) of interest.

4. Construct and evaluate intermedia transfer factors relating time-varying exposure media concentrations to time-varying environmental media concentrations.

5. Divide the population(s) of interest into an appropriate set of cohorts.

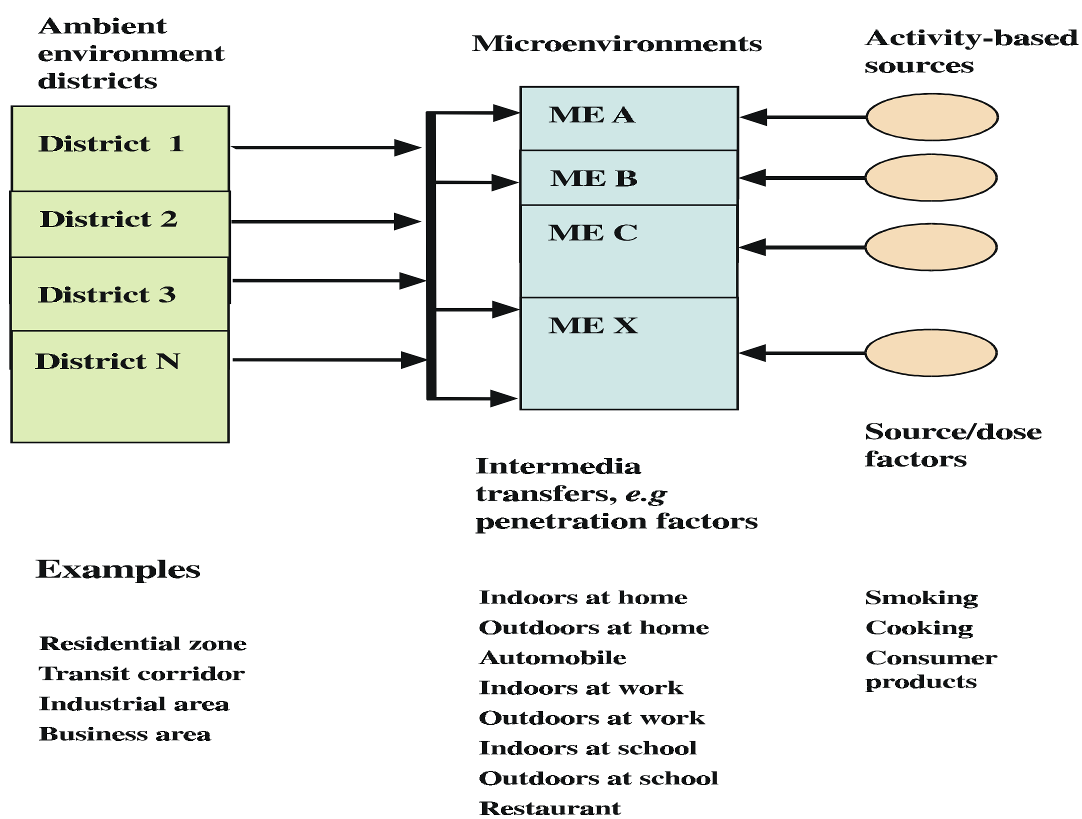
6. Develop a sequence of exposure events linking the cohorts to exposure media.

7. Create a dose profile for each exposure route based on the intake of pollutant(s) in each exposure event for each cohort.

Figure 4-3 illustrates a typical TRIM.Expo application. Pollutants from environmental media contained in environmental districts are linked to microenvironments through the intermedia transfer factors. Cohort activities are linked to the microenvironments as well. This information is then used to assess an exposure profile and/or cumulative intake during a defined time period. These steps are described in more detail below.

Figure 4-3
Sequence of Exposure Events for a Set of Population Cohorts

Illustration of the Process by which Environmental Media Concentrations for Multiple Exposure Districts are linked using Intermedia Transfers to Exposure Media in a Set of Microenvironments



4.2.1 DEFINE STUDY AREA, EXPOSURE DISTRICTS, AND ENVIRONMENTAL MEDIA

A study area is an urban and/or local area for which environmental concentrations have been assembled for an exposure assessment. It is divided into one or more exposure districts. In order to perform multimedia exposure assessments, concentration data from multiple environmental media (*i.e.*, ambient air, vegetation, surface soil, root zone soil, deeper or vadose zone soil, ground water, surface water) are needed for each exposure district. The concentration information is gathered either from analysis of ambient monitoring data or from a simulation model such as TRIM.FaTE. Each ambient environmental medium is characterized in terms of one or more component phases – gas, water, liquid, and/or solids. Each environmental medium is described below.

4.2.1.1 Ambient Air

The ambient (*i.e.*, outdoor) air in an exposure district can be characterized in terms of its gas, particulate matter, and water composition. Its volume and mass are defined by the area of the exposure district and the depth of the lower troposphere. Pollutants in ambient air are dispersed by atmospheric advection and diffusion and are influenced greatly by meteorological parameters. Because particle size influences the particle's behavior in the atmosphere with respect to deposition and settling and its ability to penetrate the lung cavities and affect human health, it is important to consider particulate matter of various cut sizes, such as PM_{10} and $PM_{2.5}$. The TRIM.Expo module will consider other particle sizes, as the need arises, in the future. In addition, during precipitation (*e.g.*, rain, snow) and fog events, it is important to characterize the volume fraction of air that is water.

4.2.1.2 Vegetation

Vegetation is the dominant component of the terrestrial plants exposure district. Vegetation generally has contact with two other environmental media, air and soil. However, plant interactions with these media are not understood well enough to define an accurate method for predicting pollutant uptake. In order to assess potential vegetation-pathway exposures, vegetation can be further delineated into above-ground vegetation and root crops. Above-ground vegetation includes leafy vegetables (*e.g.*, cabbage, cauliflower, broccoli), exposed produce (*e.g.*, apples, berries, cucumber, squash), protected produce (*e.g.*, citrus fruits), and grains (*e.g.*, wheat, corn, rice). Root crops include, for example, carrots, beets, legumes, and melons.

4.2.1.3 Surface Soil

Surface soil consists of solid, liquid, and gas phases. Studies of radioactive fallout in agricultural land management units reveal that, in the absence of tilling, particles deposited from the atmosphere accumulate in and are resuspended from a thin ground or surface soil layer with a thickness in the range 0.1 to 1 cm (Whicker and Kirchner 1987). The ground-surface-soil layer, has a lower water content and higher gas content than underlying layers.

4.2.1.4 Root Zone Soil

Root zone soil consists of solid, liquid, and gas phases. Soil-water content in the root-zone is somewhat higher than that in surface soils because the presence of clay serves to retain water. The roots of most plants are confined within the first meter of soil depth. In agricultural lands, the depth of plowing is 15 to 25 cm. In addition, the diffusion depth, which is the depth below which a pollutant is unlikely to escape by diffusion, is on the order of 1 m or less for all but the most volatile pollutants.

4.2.1.5 Vadose Zone Soil

Vadose zone soil has solid, liquid, and gas phases. The soil in this layer typically has a lower organic carbon content and a lower porosity than the root zone soil. It is assumed that pollutants in this layer will move downward to the ground water zone primarily by capillary motion of water and leaching.

4.2.1.6 Ground Water

Ground water is defined as water that can be withdrawn from the saturated zone below the vadose zone of the soil layer. Ground water consists of both a liquid and a suspended particle phase.

4.2.1.7 Surface Water

Surface water is composed of two phases: pure water and suspended sediment material. The suspended sediment material phase contains sorbed pollutants. Surface water compartments are assumed to be well-mixed systems and include ponds, lakes, creeks, rivers, estuaries, seas, and oceans.

4.2.2 DEFINE EXPOSURE MEDIA AND MICROENVIRONMENTS

The exposure assessment process consists of relating pollutant concentrations in the environmental media (*e.g.*, ambient air, surface soil, ground water) to pollutant concentrations in the exposure media with which a human population has contact (*e.g.*, personal air, tap water, foods, household dusts). The exposure media that have been identified for inclusion in TRIM.Expo include the following.

- Outdoor air;
- Indoor air;
- Tap water;
- Home-grown food (*i.e.*, produced by and consumed by a household);

- Locally-produced food (*i.e.*, produced by home gardens and commercial farms in contact with air, soil, and/or water in the study area);
- Prepared food;
- Breast milk;
- House dust;
- Soil;
- Swimming pools; and
- Recreational surface water.

Microenvironments are locations in which a population comes into contact with pollutants. They are well-characterized, relatively homogenous locations with respect to pollutant concentrations for a specified time period. Table 4-1 is an initial list of the microenvironments that will be included in TRIM.Expo., other microenvironments will be added during the course of module development.

Table 4-1
Microenvironments to be Included in TRIM.Expo

Microenvironment #	Microenvironment	
	General	Specific
1	In vehicle	Car
2	In vehicle	Bus
3	In vehicle	Truck
4	In vehicle	Other
5	Indoors	Public garage
6	Outdoors	Parking lot/garage
7	Outdoors	Near road
8	Outdoors	Motorcycle
9	Indoors	Service station
10	Outdoors	Service station
11	Indoors	Residential garage
12	Indoors	Other repair shop
13	Indoors	Residence - no CO source
14	Indoors	Residence - gas stove
15	Indoors	Residence - attached garage

Microenvironment #	Microenvironment	
	General	Specific
16	Indoors	Residential - stove and garage
17	Indoors	Office
18	Indoors	Store
19	Indoors	Restaurant
20	Indoors	Manufacturing facility
21	Indoors	School
22	Indoors	Church
23	Indoors	Shopping mall
24	Indoors	Auditorium
25	Indoors	Health care facility
26	Indoors	Other public building
27	Indoors	Other location
28	Indoors	Not specified
29	Outdoors	Construction site
30	Outdoors	Residential grounds
31	Outdoors	School grounds
32	Outdoors	Sports arena
33	Outdoors	Park/golf course
34	Outdoors	Other location
35	Outdoors	Not specified
36	In vehicle	Train/subway
37	In vehicle	Airplane

4.2.3 DEFINE RELEVANT INTERMEDIA TRANSFERS

An intermedia transfer factor is an algorithm that expresses the transfer of a pollutant from an environmental medium to an exposure medium. The following tables summarize intermedia transfers which need to be considered in exposure modeling. Some of these intermedia transfers, where feasible and appropriate, will be included in TRIM.Expo, while others may be addressed within the TRIM.FaTE module. Each cell representing an interaction is shaded, and the exposure pathways (*i.e.*, inhalation, ingestion, dermal contact) that results from the intermedia transfer is indicated. The tables below show the matrix of links between the various exposure media noted above and ambient-air phases (Table 4-2), ambient soil media (Table 4-3), ambient water media (Table 4-4), and ambient vegetation (Table 4-5).

Table 4-2
Matrix of Links Between Ambient-Air Phases and Various Exposure Media

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Ambient air			
	Gas Phase	$PM_{2.5}$	PM_{10}	Precipitation
Outdoor Air				
gases	Inhalation			
$PM_{2.5}$		Inhalation		
PM_{10}			Inhalation	
precipitation				
Indoor Air				
gases	Inhalation			
$PM_{2.5}$		Inhalation		
PM_{10}			Inhalation	
water vapor				
House Dust				
on floors		Ingestion/dermal	Ingestion/dermal	
on surfaces		Ingestion/dermal	Ingestion/dermal	
Soil				
Water				
Food				
home fruits				
protected				
unprotected	Ingestion	Ingestion	Ingestion	Ingestion
home vegetables				
above ground	Ingestion	Ingestion	Ingestion	Ingestion
root crops				
home grains	Ingestion	Ingestion	Ingestion	Ingestion
meat	Ingestion	Ingestion	Ingestion	
milk	Ingestion	Ingestion	Ingestion	
dairy products	Ingestion	Ingestion	Ingestion	
eggs	Ingestion	Ingestion	Ingestion	
breast milk	Ingestion	Ingestion	Ingestion	
prepared foods				

Table 4-3
Matrix of Links Between Soil Media and Various Exposure Media

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Soil		
	Surface Soil	**Root Zone Soil**	**Vadose Zone Soil**
Outdoor Air			
gases	Inhalation	Inhalation	
$PM_{2.5}$	Inhalation		
PM_{10}	Inhalation		
precipitation			
Indoor Air			
gases	Inhalation	Inhalation	Inhalation
$PM_{2.5}$	Inhalation		
PM_{10}	Inhalation		
water vapor			
House Dust			
on floors	Ingestion/dermal		
on surfaces	Ingestion/dermal		
Soil			
residential	Ingestion/dermal	Ingestion/dermal	
construction site	Ingestion/dermal	Ingestion/dermal	
industrial site	Ingestion/dermal		
agricultural site	Ingestion/dermal	Ingestion/dermal	
recreational site	Ingestion/dermal		
school	Ingestion/dermal		
Tap Water			
Swimming Pool			
Surface Water used for Recreation			
Food			
home fruits			
protected		Ingestion	
unprotected	Ingestion	Ingestion	
home vegetables			
above ground	Ingestion	Ingestion	
root crops			

EXPOSURE MEDIA		ENVIRONMENTAL MEDIUM = Soil		
		Surface Soil	Root Zone Soil	Vadose Zone Soil
	home grains	Ingestion	Ingestion	
	meat	Ingestion	Ingestion	
	milk	Ingestion	Ingestion	
	dairy products	Ingestion	Ingestion	
	eggs	Ingestion	Ingestion	
	breast milk	Ingestion	Ingestion	
	prepared foods			

Table 4-4
Matrix of Links Between Water Media and Various Exposure Media

EXPOSURE MEDIA		ENVIRONMENTAL MEDIUM = Water			
		Surface Water		Ground Water	
		Liquid Phase	Particle Phase	Liquid Phase	Particle Phase
Outdoor Air					
Indoor Air					
	gases	Inhalation		Inhalation	
	$PM_{2.5}$				
	PM_{10}				
	water vapor	Inhalation		Inhalation	
House Dust					
Soil					
	residential	Ingestion/dermal		Ingestion/dermal	
	construction site	Ingestion/dermal		Ingestion/dermal	
	industrial site	Ingestion/dermal		Ingestion/dermal	
	agricultural site	Ingestion/dermal		Ingestion/dermal	
	recreational site	Ingestion/dermal		Ingestion/dermal	
	school	Ingestion/dermal		Ingestion/dermal	
Tap Water		Ingestion/dermal	Ingestion	Ingestion/dermal	Ingestion
Swimming Pool		Ingestion/dermal		Ingestion/dermal	
Surface Water used for Recreation		Ingestion/dermal	Ingestion	Ingestion/dermal	Ingestion
Food					

EXPOSURE MEDIA	**ENVIRONMENTAL MEDIUM = Water**			
	Surface Water		**Ground Water**	
	Liquid Phase	Particle Phase	Liquid Phase	Particle Phase
home fruits				
protected	Ingestion		Ingestion	
unprotected	Ingestion		Ingestion	
home vegetables				
above ground	Ingestion		Ingestion	
root crops	Ingestion		Ingestion	
home grains	Ingestion		Ingestion	
meat	Ingestion		Ingestion	
milk	Ingestion		Ingestion	
dairy products	Ingestion		Ingestion	
eggs	Ingestion		Ingestion	
breast milk	Ingestion		Ingestion	
prepared foods	Ingestion	Ingestion	Ingestion	Ingestion

Table 4-5
Matrix of Links Between Vegetation and Various Exposure Media

EXPOSURE MEDIA		ENVIRONMENTAL MEDIUM = Vegetation			
		Above-Ground Plants			Root Crops
		Fruits	Vegetables	Grains	Crops
Outdoor Air					
Indoor Air					
House Dust					
Soil					
Water					
Food					
	home fruits				
	protected	Ingestion			
	unprotected	Ingestion			
	home vegetables				
	above-ground		Ingestion		
	root crops				Ingestion
	home grains			Ingestion	
	meat	Ingestion	Ingestion	Ingestion	Ingestion
	milk	Ingestion	Ingestion	Ingestion	Ingestion
	dairy products	Ingestion	Ingestion	Ingestion	Ingestion
	eggs			Ingestion	Ingestion
	breast milk	Ingestion	Ingestion	Ingestion	Ingestion
	prepared foods	Ingestion	Ingestion	Ingestion	Ingestion

4.2.4 DIVIDE POPULATION INTO APPROPRIATE SETS OF COHORTS

The first step in selecting population(s) of interest is to define the total population associated with all of the exposure districts. This may be expanded to incorporate more than residents of the defined exposure districts. For example, people who do not reside within the exposure district but consume its agricultural products or fish may be included. Once the population(s) are identified, the second step is to decide whether to include all of the population members in a region or a subset of the population of concern due to a demographic factor, activity, or health characteristic (*e.g.*, asthmatics, outdoor workers, pregnant women).

The population of interest is then divided into cohorts. In TRIM.Expo, each individual is exclusively assigned to a single cohort. Cohorts are distinguished from the overall population based on attributes including age, gender, health status (*e.g.*, asthmatics), exposure district, and housing types (*e.g.*, gas stoves, HVAC systems). The number of cohorts selected depends largely on the level of resolution of the exposure factor data used to characterize the population and on the level of exposure resolution required. The type of pollutants and sources under consideration can affect the number and type of cohorts as well.

As previously stated, cohorts can be defined for a particular application or situation. For example, cohort exposure can be a function of demographic group, location of residence, location of work place, and type of home ventilation system. Cohort exposure can be linked to ambient pollutant concentrations in multiple districts (*e.g.*, home and work district). Specifying the demographic group allows cohort exposure to be linked to activity patterns that vary with age, work status, and other demographic variables. In some analyses, cohorts are further distinguished according to time spent in particular microenvironments. For example, in studies of ozone exposures, additional cohorts were created to account for children who spent significant amounts of time outdoors and also for adults who worked outdoors. These cohort designations helped analysts estimate exposures for subgroups in the population with the greatest potential for higher exposures.

4.2.5 DEVELOP AN EXPOSURE-EVENT SEQUENCE FOR EACH COHORT

Once a set of cohorts has been selected, a sequence of exposure events is defined for each cohort. An exposure-event sequence is a chronological set of events that define the activity/time allocation of each cohort. An exposure-event sequence defines a cohort by (1) exposure district, (2) microenvironment, and (3) activity at each time step of a calculation. Implicit in the definition of activities for the exposure-event sequence is information about the time of year or season, through the selection of activity patterns based on the outdoor air temperature that coincided with the collection of the activity pattern data. The following example in Table 4-6 shows simple eight-hour exposure-event sequence. Because an exposure-event sequence is developed from an individual's activity pattern data used to represent the cohort, concentrations in each of the microenvironments are the same for each member of the cohort. Multiple runs of the model results in variation of the activity patterns for a given cohort.

Table 4-6
Sample Eight-Hour Exposure-Event Sequence

Time:	06:00	07:00	08:00	09:00	10:00	11:00	12:00
Exposure District							
Zone 1		Zone 2					
Microenvironment							
Indoors at home		Inside a vehicle	Indoors at work				
Activity							
Sleeping	Dressing, eating	Comm-uting	Working at desk				Eating lunch

4.2.6 DETERMINE EXPOSURE MEDIA CONCENTRATIONS AND CONTACT IN EACH MICROENVIRONMENT

Once a sequence of exposure events is established, the exposure medium concentration and the rate of contact between the cohort and the exposure medium in the various microenvironments must be estimated. The route of contact/intake can greatly influence the affected populations or the populations of interest that are studied in an exposure assessment. For example, hand-to-mouth contacts are more important for a population of children than for a population of adults. This information is then used to establish an exposure concentration profile, a cumulative intake, or an average exposure medium concentration over a defined averaging time.

4.2.7 ESTIMATE AN INTAKE RATE FOR EACH DOSE EVENT

For each exposure event in the exposure-event sequence, TRIM.Expo estimates the intake rate of the pollutant for all relevant routes of exposure. Initially, TRIM.Expo will provide estimates for inhalation and ingestion only. To estimate the intake rate of a pollutant via inhalation, TRIM.Expo defines each exposure with a pollutant concentration and a ventilation rate indicator. The applied dose is a function of the pollutant concentration in contact with the individual or cohort, the activities that the individual or cohort are engaged in that affects breathing rate, and the ventilation rate value that is assigned to the exposure event. Section 5.1.5 describes in detail how pollutant concentrations and the ventilation rate associated with each exposure event will be estimated.

For ingestion, TRIM.Expo estimates the average daily potential dose (ADD) for many different ingestion pathways and media of exposure. The ADD represents the amount of pollutant that enters the mouth of the exposed individual or cohort over a defined exposure event for a defined exposure duration. Data are provided on the rate of ingestion of the exposure medium (*e.g.*, water, soil, food) during an exposure event and are used to calculate the ADD. Section 6.1 provides a summary of the general approach used to characterize the ADD for an exposure medium. Subsequent sections in Chapter 6 provide details on how the algorithm applies to specific exposure media.

4.2.8 EXTRAPOLATE THE COHORT EXPOSURES TO THE POPULATIONS OF INTEREST

After the exposures to the cohorts have been calculated, they are extrapolated to the population at risk by estimating the population size for each cohort. Population estimates assigned to each cohort are calculated for both commuting (*i.e.* to work, to school) and non-commuting cohorts. The first step is to calculate the population of each demographic group that resides in a particular home district through data available from the Bureau of the Census. This information provides the population of all non-commuting cohorts by home district.

The population of non-commuting cohorts can be further divided to account for a particular attribute shared by the cohorts. The attribute should be one for which data about the size of the population can be obtained. The population size of each demographic group listed as having attribute *b* is calculated through the following equation:

$$pop(dg,ca,b) = f(ca,b) \times pop(dg,ca) \quad (4\text{-}11)$$

where:

pop(dg,ca,b)	=	The population of demographic group *d* in census area[1] *ca* having The attribute of interest *b*.
f(ca,b)	=	Fraction of people in census area *ca* that have attribute *b*.
pop(dg,ca)	=	Total number of people in demographic group *d* that reside in census area *ca*.

The values of *pop(dg,ca,b)* are summed over each home district to yield estimates of *pop(dg,h,b)*, the number of people in demographic group *dg* within home district *h* that share attribute *b*. Any number of attributes can be used to calculate *pop(dg,h,b)* if census area data are available.

The value of *pop(dg,h,b)* provides an estimate of the population in each non-commuting cohort associated with demographic group *d*g residing in home district *h* that shares the attribute of interest *b*. Next, the populations of the commuting cohorts in demographic group *dg* who share attribute *b* are calculated using the fraction of all commuters residing in home district *h* who travel to commute district *w* (including children who commute to school) using Equation 4-12:

[1] "Census area" can be any spatial area designated by the Bureau of the Census. For most exposure applications, the census tract designation is used.

$$com(dg,h,w,b) = pop(dg,h,b) \times com(h,w) / com(h) \qquad (4\text{-}12)$$

where:

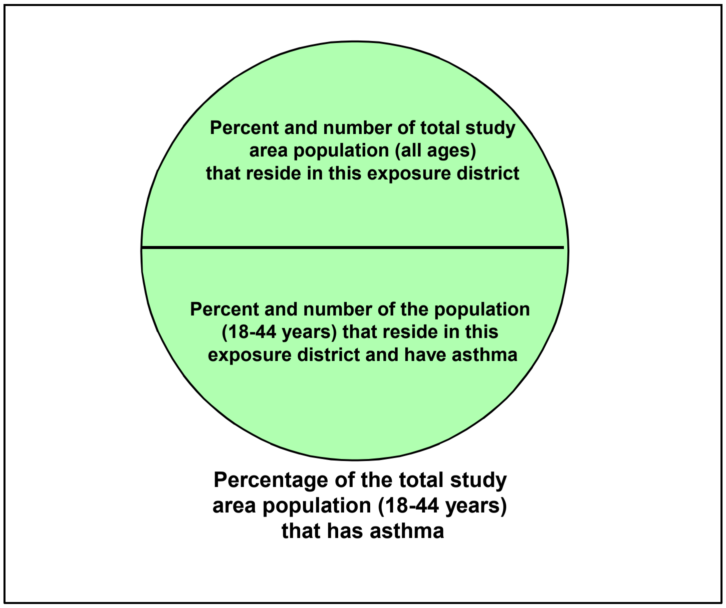
com(dg,h,w,b)	=	number of people in a commuting cohort associated with demographic group *dg* in home district *h* and commute district *w* having attribute *b.*
com(h,w)	=	number of commuters in all demographic groups that travel from home district *h* to commute district *w.*
com(h)	=	total number of commuters in home district *h*.

Estimates of *com(h)* can be obtained from census data specific to each district.

By defining cohorts according to attributes that are important to specific applications or situations, TRIM.Expo is able to extrapolate the cohort exposures to the general population while still retaining information about the incidence of exposure to the specific subset of the population under study. For example, suppose that the population of interest was individuals, ages 18 to 44, who experience asthma. For a particular study area, information for both of these attributes is available. Census data contains the breakdown of age information by location, while information on the incidence of asthma is available from various sources, including the National Center for Health Statistics and state and local health agencies. In this case, the TRIM.Expo analysis would be arranged to capture the demographic characterization of this subset of the population by selecting a demographic group that includes individuals from 18 to 44 years of age. The fraction of the demographic group with asthma can be determined from health data. When combined, this information provides an estimate of the exposures to this specific segment of the population for each exposure district, assuming that activity patterns for asthmatics do not differ significantly from those of the other members of the demographic group. Once the exposures of this sensitive subpopulation are known for each exposure district, the exposures can be readily extended to encompass the entire study area under investigation.

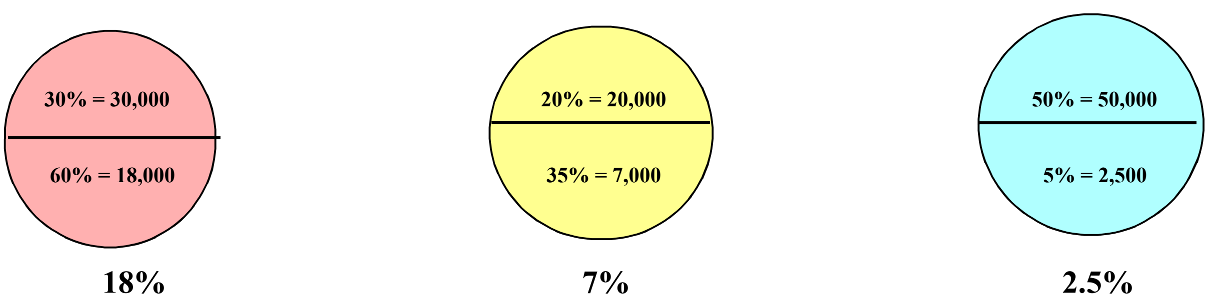
In the simple example given above, the fraction of the total population with the specified attribute in a particular exposure district can be quite different from the fraction of all people in the study area contained within that exposure district. Consider, for example, Figure 4-4 which presents a hypothetical illustration of the example above. In this figure, each circle represents an exposure district. The study area for this example is the sum of the three exposure districts. The total population of this hypothetical study area is 100,000 people. The fraction and number of the total study area population residing in each exposure district is indicated in the top half of each circle. The fraction and number of the 18 to 44 year olds in the study area population with asthma in each exposure district is indicated in the bottom half of each circle. As can be seen in this example, exposure district #3, which includes 50 percent of the total population of the study area, contains 2,500 people age 18 to 44 with asthma, only 2.5 percent of the total study area population (*i.e.*, all three exposure districts combined). However, exposure district #2, which includes only 20 percent of the total population of the study area, accounts for 7 percent (7,000) of the cases of asthma in the 18 to 44 year-olds in the study area. Finally, exposure district #1, which has one-third of the study area's total population, has 18,000 cases of asthma in people of age 18 to 44, 18 percent of the total study area population.

Figure 4-4
Hypothetical Spatial Distribution of the Incidence of Asthma



SCENARIO:
Study area population (all ages) = 100,000
Study area population (18-44 years) that has asthma = 27,500 (27.5 percent)

Exposure District 1 **Exposure District 2** **Exposure District 3**



The example above illustrates that the spatial distribution of a demographic variable, such as the incidence of a particular disease, is not necessarily the same as the spatial distribution of the general population. The illustration also points out that conducting exposure analyses on a smaller spatial scale is likely to lead to more accurate results. This is particularly true when investigating exposures related to factors that have a high degree of variability over small distances. Different exposure estimates for the sensitive subpopulation of individuals suffering from asthma would have been obtained if the exposures of the entire population were calculated and then adjusted for the incidence of asthma based on the percentage of reported cases for the study area as a whole without regard for the spatial variation of this disease.

4.2.9 FUNCTIONAL ATTRIBUTES

The TRIM.Expo module will include important attributes that are needed by analysts and decision-makers to investigate the complex nature of multipollutant and multipathway human exposures to hazardous and criteria air pollutants in the environment. This section briefly describes many of the functional attributes that will be included in TRIM.Expo. The attributes fall into two major categories: (1) important considerations related to the scientific defensibility of the exposure estimates, and (2) design features of TRIM.Expo that help ensure the needed flexibility and ease of use of the modeling system.

4.2.9.1 Inclusion of Indoor and Outdoor Environments and Their Emission Sources

Recent studies have shown the importance of including both indoor and outdoor environments when assessing human exposures to toxic pollutants (Ozkaynak et al. 1996, U.S. EPA 1987, Wallace et al. 1985, Wallace et al. 1991). These studies called the Total Exposure Assessment Methodology (TEAM) and Particle Total Exposure Assessment Methodology (PTEAM) studies, and other indoor/outdoor studies that have succeeded them, reported that indoor concentrations of many toxic air contaminants were often greater than concurrent outdoor concentrations. Other studies have reported that most people in the U.S. can spend as much as 90 percent of their time indoors or inside motor vehicles (Jenkins et al. 1992, U.S. EPA 1996a). Conversely, exposures to the NAAQS pollutants (*e.g.*, ozone, sulfur dioxide) are dominated by outdoor levels or by ambient air that infiltrates to indoor environments. Therefore, it is vital that a framework for assessing the total human exposure to pollutants include the indoor, in vehicle, and outdoor environments.

An important microenvironment for exposure to multiple airborne pollutants is inside a passenger vehicle. This microenvironment is treated similarly as the indoor environment, although a significant fraction of the concentration found indoors may come from penetration of ambient air. Nevertheless, exposures to many pollutants within a moving vehicle have been reported to be higher than either roadside or ambient (*i.e.,* away from a road) exposures (CARB 1998b). Lawryk et al. (1995) reported that commuting can account for a substantial amount of a person's daily exposure to select toxic pollutants. Furthermore, both studies reported that many factors can affect the levels of pollutants inside a vehicle, including the general condition and maintenance of the vehicle, the vehicle's age, the density of the surrounding traffic, and the resulting effect these factors have on the speed of the vehicle.

Besides traveling in a vehicle, other activities that can have a significant impact on exposures are cooking and smoking. Increased concentrations in close proximity to gas stoves have been reported for NO_2 (Sega and Fugas 1991), CO (U.S. EPA 1984), and $PM_{2.5}$ and PM_{10} (Ozkaynak et al. 1996). The concentrations of other pollutants produced through incomplete combustion have also been found to be higher close to a cooking appliance. Ozkaynak et al. (1996) also reported that smoking was a significant source of particles in homes in the PTEAM study. They found that homes where smoking was reported averaged approximately 30 $\mu g/m^3$ higher levels of PM_{10} than homes without smoking. Numerous other exposure studies have reported higher concentrations of CO, particles, and toxic pollutants in indoor environments (particularly the home) with environmental tobacco smoke (ETS) (Daisey et al. 1998, Jenkins et al. 1996, Miller et al. 1998, Phillips et al. 1998, Quackenboss et al. 1991, Thomas et al. 1993, Waldman et al. 1991).

The TRIM.Expo module has several indoor and in-vehicle microenvironments, including inside a home (several different locations); in transit (*e.g.*, automobiles, buses, trains), indoors at work or school; indoor recreational facilities (*e.g.*, movie theaters), shopping malls, and restaurants. In addition, TRIM.Expo has the flexibility to include other indoor microenvironments of importance as information becomes available.

While evidence continues to accumulate regarding the importance of indoor sources and environments on exposures, there remains important sources of exposure outdoors, too. In fact, studies show that in the absence of indoor sources, penetration of outdoor pollutants were responsible for elevated indoor concentrations (see, for example, Lioy et al. 1991). However, investigations into the sources of outdoor pollutants have found that, although human activities, such as motor vehicle use have a major impact on ambient levels of particles and toxic pollutants, relatively small, local sources of specific toxic pollutants such as repair shops can also have a significant impact on the exposures to a nearby population. Moreover, exposures to pollutants from certain outdoor sources can be affected by local climatology, thereby exhibiting seasonal variations in the exposure profile. An example are pollutants that are emitted by the burning of heating fuel in the winter months (Lioy and Daisey 1990).

The TRIM.Expo module currently has several outdoor environments included in its modeling system. There are outdoor microenvironments specified for at home, in transit (*e.g.,* walking, bicycling), at work, and recreational locations. The location where eating takes place may also be important for estimating ingestion exposures.

4.2.9.2 Flexible, Modular, and Portable Algorithms

The TRIM.Expo module is designed with features that will facilitate future expansion and integration of the framework in anticipation of new modeling techniques and data. Additionally, there is a need for TRIM.Expo to be compatible with other exposure modeling platforms developed both within and outside of EPA. The design features that will allow for these capabilities are portability, modularity, and flexibility. These three features are all interrelated in function and purpose. They follow the recommended guidance set forth by the National Research Council's *Committee on Advances in Assessing Human Exposure to Airborne Pollutants* (NRC 1991b). Flexibility means that the model algorithms are written using precise, standard encoding practices. This approach will allow the model to be updated relatively easily as new data and new modeling techniques become available. The TRIM.Expo module algorithms are being designed to readily incorporate new information regarding both data and methods. As an example, comments will be included within the model's source code which will help future developers understand how the model was constructed and explain each of the functional components of the model. This seemingly minor point has important implications for the future development of TRIM.Expo because (1) model development and revisions may continue indefinitely, and (2) responsibility for future updates of the model may shift to different groups.

Another aspect of flexibility is the use of modular design in model development. Modular design, as its name implies, means that the components of the model involved in the computation of exposures are separated into discreet units, where each unit is responsible for a particular function. These discreet units, or modules, are called upon during the execution of a model run to perform a specific function or set of functions. If a particular application does not require the function(s) performed by a certain module, then the calculations or routines performed by the module are not called upon. In most of the early exposure models, all of the functions of a model were executed regardless of whether they were required for the particular application. Using only the modules that are needed for a specific application reduces the amount of computer resources required. Using a modular approach also aids in the development of the model because when specific model functions are in modules, they can be revised and tested without running the entire model. This makes isolating and correcting mistakes in the model's algorithms easier, as well.

The functional attribute of portability is important to the development of the TRIM.Expo modeling system. Portability refers to how easily the model can be integrated with other modeling systems such as Models-3 or MENTOR, in the case of TRIM. Expo. The overall goal of systems such as Models-3 and MENTOR is to simplify and integrate the development and use of complex environmental models. The developers of these systems seek to provide a set of ready-to-use methodological tools and linkages to relevant databases for performing assessments of exposure. Hence, it is important that TRIM.Expo can take full advantage of the designs and numerical analysis tools provided by these systems. Therefore, TRIM.Expo is based on an open, user-oriented implementation that is compatible with the components of other modeling systems. An open system design means that TRIM.Expo's development is not specific to a single computing platform. Finally, TRIM.Expo can be run without the use of proprietary software or model components, enhancing both the flexibility and portability of TRIM. Expo.

4.2.9.3 Explicit Treatment of Uncertainty and Variability

While the importance of characterizing uncertainty and variability explicitly and separately is well recognized (NAS 1994, CRARM 1997, U.S. EPA 1997c), OAQPS intends to *selectively* apply uncertainty and variability analyses on a case-specific basis, (*i.e.*, for critical parameters and, where appropriate, based on the underlying science and data).

The TRIM.Expo module explicitly treats the uncertainty in the model estimates of exposure. Uncertainty is the lack of knowledge of the actual values of physical variables (parameter uncertainty) and of physical systems (model uncertainty). For example, parameter uncertainty results when non-representative sampling (to measure the distribution of parameter values) gives sampling errors. Model uncertainty also results from simplification of complex physical systems. Uncertainty can be reduced through improved measurements and improved model formulation.

As with uncertainty, the variability in model inputs will be explicitly characterized in TRIM.Expo, wherever feasible. Variability is not to be confused with uncertainty; they are two separate aspects inherent in data sampled from a population. Variability represents the diversity or heterogeneity in a population or parameter and is sometimes referred to as natural variability. An example is the variation in the heights of people. Variability cannot be reduced by using more measurements or measurements with increased precision (*i.e.*, more precise measurements of people's heights does not reduce the natural variation in their heights). However, it can often be reduced by a more detailed model formulation. For example, modeling people's heights in terms of their age will reduce some of the unexplained variability in the distribution of data on heights. Variability among the members of a population in factors such as food ingestion rates, exposure duration, and expected lifetime can be described by purely stochastic (*i.e.*, involving chance or probability) processes. These processes are random or variable and are not characterized by a single value but can be described by a distribution. Thus, estimation of the moments of the distribution (*e.g.*, mean, variance, skewness) is possible.

The TRIM framework includes an approach to estimate uncertainty and variability in a manner that allows for integration between the TRIM modules while tracking the uncertainty and variability through the modules. The remainder of this section briefly describes the approach for estimating uncertainty and variability. For a more rigorous explanation on uncertainty and variability and implemention in the TRIM framework, please refer to the 1999 TRIM Status Report (U.S. EPA 1999c).

The EPA chose a staged approach for analyzing uncertainty and variability since it has several advantages for models as complex as TRIM. The first stage, which is comparatively easy to implement, is known as a sensitivity and screening analysis. This stage involves identifying influential parameters and developing an importance-ranking of parameters to focus and reduce the number of parameters analyzed in the uncertainty and variability analysis. The sensitivity and screening analysis computes the importance of parameters by calculating the extent to which model results change when parameters are varied singly or in pairs. This process provides for a first-order determination of the most influential parameters and allows further analysis to focus on the key parameters. Furthermore, this screening approach narrows down the scope of the detailed analysis in the second stage and reduces the number of parameters by identifying influential parameters that should be retained for further analyses. This is a critical step toward the goal of producing an economical representation of uncertainty and variability by excluding unnecessary terms and parameters and still capturing all of the significant features of model uncertainty and variability.

The second stage of TRIM.Expo's uncertainty and variability analysis is more complex and involves a Monte Carlo approach. Monte Carlo methods analyze model uncertainty by using statistical sampling techniques to estimate statistics that characterize uncertainty. Essentially, a

Monte Carlo approach entails performing many model runs with model inputs that are randomly sampled from specified distributions for the model inputs. These can be set up to characterize the propagation of uncertainty and variability of the model input parameters, taking into account distributions of parameter uncertainty and variability and parameter dependencies. These simulations provide uncertainties of model outputs in terms of distributions of model outputs, joint distributions of model inputs and outputs, and summary scalar measures (*i.e.*, the core data from which information about uncertainty and variability can be extracted).

This two-stage analysis of uncertainty and variability will be performed for each of the TRIM modules to study the propagation of uncertainty. The Monte Carlo simulations for each TRIM module will be performed sequentially in the order that the TRIM modules are run. Sufficient information must be transmitted from one module to the next to be able to propagate distributional information to succeeding Monte Carlo simulations. Since the amount of data produced from Monte Carlo simulations is voluminous, the full results will be archived and a reduced set will be retained as input for the next module. The output values from each of the TRIM modules as well as the model inputs (*i.e.,* parameter values) for each Monte Carlo simulation will be saved and can be passed along to the next module for subsequent uncertainty analysis. However, the amount of data would increase drastically from one module to the next. Therefore, it is important to track the input parameters to each TRIM module.

To reduce the size and complexity of the transfer of uncertainty and variability information between TRIM modules, the results can be summarized in the form of non-parametric probability distributions that can be passed to the next module, where each distribution to be passed is characterized non-parametrically by its percentiles.

The screening stage described above involves a sensitivity ranking analysis to select the critical parameters to be tracked for the more detailed uncertainty analysis; all other parameters would be set at their central tendency value. This focus on critical parameters also decreases the amount of information to be tracked. To further reduce the volume of information, after summarizing the results from one module as probability distributions, the transmission of information to the next module is filtered to select the most critical parameters (*e.g.*, those that account for 95 percent of the variance of the uncertainty and variability).

It is important to note that since data for many of the input variables in TRIM.Expo (*e.g.*, time-activity patterns, ventilation rates, air exchange rates) are not available to cover the entire range of possible values, Monte Carlo simulations are used to better represent the distribution of exposures that occur among the people in an exposure assessment. While this method better captures the variability of the population’s exposures, it underestimates the repetitive nature of certain high exposure situations (*e.g.*, long commutes in slow-moving traffic or preparing foods in a manner that increases the release of toxic pollutants) for certain segments of the population.

Furthemore, it should be noted that much of the data used to characterize variability related to exposure, such as time-activity patterns or other exposure factors are sometimes based on short-term (multiday) measurements (*e.g.*, diary studies, recall, monitoring). Despite the limitations and assumptions built into using such data to generate long-term factors, OAQPS believes that these data are the best available and extrapolating to generate long-term factors or creating a longer term sequence of such data is the best approach. It should be reiterated that TRIM, due to its architecture, is a dynamic modeling system, not a static model, and will be able to undergo frequent updates that reflect new science and information. Therefore, once alternative and improved approaches (*e.g.*, correlated diaries for activity and consumption information at the individual level developed through statistical analysis of multiday diaries) become available, they will be evaluated and incorporated into TRIM where appropriate.

4.3 DATA INPUT REQUIREMENTS

Inputs to TRIM.Expo include environmental media concentrations, intermedia transfer factors, and/or the input needed to calculate intermedia transfers from algorithms, cohort activity data, and demographic and at-risk population data. The sections below summarize the principle sources of input data in these areas.

Although TRIM.Expo is primarily a stochastic model, distributions for many of the model's inputs are either not available or are incomplete. Through the use of a systematic sensitivity analysis, exposure pathways and parameters can be identified by the model that do not make a major contribution to the assessment endpoint nor to the overall uncertainty and variability. The use of point estimates can then be considered for these parameters (U.S. EPA 1997c). Conversely, TRIM.Expo will use Monte Carlo analysis for those parameters that are found to have a significant impact on exposure and that have data available. Hence, assessments in TRIM.Expo will be able to use a combination of distributional data for input parameters that are judged to be important by the analyst, and point estimates for those parameters that are either determined to contribute little to the exposure outcome or that have insufficient data available. Whichever distribution type is selected for a particular parameter, the analyst will be informed by the model of the choices made and the implications that may result.

A *probability density function* (PDF) will be developed for many of the input variables used in TRIM.Expo. For continuous random variables, the PDF expresses the probability that the random variable falls within some very small increment (U.S. EPA 1997c). It must be emphasized that distributions for many of the exposure factors in TRIM.Expo have not been developed to date, hence, a major effort is required to develop the PDFs for input to the model.

Probability density functions can be characterized by numerous distributional forms (Cullen and Frey 1999). For each TRIM.Expo application, the analyst needs to address several critical issues regarding data sorting and manipulation. These issues include, but are not limited to the following: (1) how to develop a PDF based on limited data; (2) how to set the confidence or uncertainty limit for a PDF; (3) how to truncate PDFs to eliminate unrealistic scenarios; and (4) how to use data that is below its detection limit. The EPA has convened workshops to address important issues regarding data distributions and their variability and uncertainty (U.S. EPA 1996b, U.S. EPA 1999g). The reader is urged to refer to these workshop reports for more in-depth information regarding these issues.

Another issue concerning the development and use of data inputs is that as studies provide new information on exposure factors, discrepancies may appear between the factors in one study as compared to those from a different study. This complicates the selection of exposure factors for use in TRIM.Expo. Therefore, whenever possible, the developers of TRIM.Expo will use exposure factors that are consistent across EPA program offices. Furthermore, they will draw on the efforts of, and work cooperatively with, ORD and the other program offices to determine the most appropriate exposure factors and will update these periodically to reflect the most current knowledge in this field.

4.3.1 ENVIRONMENTAL MEDIA CONCENTRATIONS

The required environmental media concentration data input for TRIM.Expo includes ambient pollution concentration estimates. For the exposure duration of interest in TRIM.Expo, a concentration profile for each of the principal environmental media (*i.e.*, air, soil, water, vegetation) included in the analysis for each exposure district is needed. Pollutant concentration data for TRIM.Expo is assumed to be available from analysis of monitoring data, from a dispersion model, or from a multimedia transport model such as TRIM.FaTE. The two environmental media for which monitoring data are most abundant are air and water.

The OAQPS is responsible for managing a monitoring network of ambient fixed-site monitors for air pollutants. The OAQPS uses this network of monitors to help ensure that the levels of the criteria pollutants (*i.e.*, carbon monoxide, nitrogen dioxide, sulfur dioxide, ozone, particulate matter, lead) do not exceed the NAAQS established to comply with the CAA. The air quality measurements are collected by monitors at thousands of sites across the nation operated by state and local environmental agencies. Each monitor measures the concentration of a particular pollutant in the air. Monitoring data indicate the average pollutant concentration during a time interval, usually one hour or 24 hours. The monitoring stations in this network are called the State and Local Air Monitoring Stations (SLAMS). To obtain more timely and detailed information about air quality in strategic locations across the nation, OAQPS established an additional network of monitors, called the National Air Monitoring Stations (NAMS). The NAMS sites, which are part of the SLAMS network, must meet more stringent monitor siting, equipment type, and quality assurance criteria.

The CAA also stipulates that each state include a comprehensive inventory of existing sources of air pollution and an accurate estimate of the total amount of pollutants (*e.g.*, VOCs) emitted to the air by each source during a calendar year. These pollutant emissions estimates are compiled by operators of industrial and commercial enterprises, state and local environmental agencies, and EPA. The amount of pollutant is calculated using EPA-approved methods and measurable factors such as the quantity of fuel used.

All of these emissions data are compiled in a single database called the Aerometric Information Retrieval System (AIRS). The AIRS contains all of the air quality, emissions, compliance, and enforcement information that OAQPS and state agencies collect to carry out their respective programs for improving and maintaining air quality.

The EPA's Office of Water (OW) manages information collected on pollutant concentrations measured in waterbodies. The data are collected from monitoring conducted at regular sites on a continuous basis, at selected sites on an as needed basis or to answer specific questions, on a temporary or seasonal basis, or on an emergency basis. The responsibility to monitor water quality rests with many different agencies. State pollution control agencies have key monitoring responsibilities and conduct vigorous monitoring programs. Many local governments, such as city and county environmental offices, also conduct water quality monitoring. In addition, other Federal agencies are also involved in water quality monitoring. For example, the U.S. Geological Survey (USGS) conducts extensive chemical monitoring through its National Stream Quality Accounting Network (NASQAN) at fixed locations on large rivers around the country.

Many agencies and organizations maintain computerized data systems to store and manage the water quality data they or others collect. Perhaps the single largest such ambient water quality data system is EPA's STORET (STOrage and RETrieval) system. Much of the data collected by state, local, and federal agencies and by some private entities such as universities and volunteer monitors are entered into STORET. Raw data in STORET can be accessed, analyzed, and summarized by many users and for many purposes.

The TRIM.Expo module will be capable of using data from multimedia transport models as input data for ambient pollutant concentrations, particularly for multimedia, multipathway pollutants. One such model is the TRIM.FaTE module. The TRIM.FaTE module can estimate pollutant concentrations in multiple environmental media and biota, and accounts for transfer of mass throughout an environmental system. It models the movement of pollutant mass over time through a bounded system, which includes both biotic and abiotic components. The boundaries of the system are defined by the user, and can easily conform to the exposure districts in a TRIM.Expo application.

4.3.2 CONCENTRATIONS OF POLLUTANTS IN MICROENVIRONMENTS

Pollutant concentrations will need to be supplied to TRIM.Expo for all microenvironments in which significant contributions to exposures occur. When measured data are unavailable, there are various techniques for estimating these microenvironmental concentrations. These techniques are discussed below, with a focus on ways of estimating microenvironmental concentrations of pollutants in air.

4.3.2.1 Indoor Versus Outdoor Concentrations

Studies that simultaneously measure indoor and outdoor concentrations of various pollutants show that numerous factors affect a pollutant's ability to penetrate to the inside of a building from outdoors (Johnson et al. 1996c). One of the most comprehensive measurement studies of indoor/outdoor concentrations of air pollutants conducted to date is the Total Exposure Assessment Methodology (TEAM) (U.S. EPA 1987). This multi-year study was conducted in the early to mid 1980's. During the study, measurements of the exposures of 600 individuals to 20 target chemicals in both air and water were made. The 600 study participants were a representative sample of a total population of 700,000 residents of cities in New Jersey, North Carolina, North Dakota, and California. One of the most important findings of the TEAM study was that personal (air) and indoor exposures to VOCs are nearly always greater than outdoor levels (Wallace et al. 1991, U.S. EPA 1987). The TEAM studies answered a question of equal importance for modeling exposures to air pollutants, that is: "Is there any indoor and outdoor relationship associated with the variation of one or more air pollutants measured simultaneously at a residence?" In the New Jersey TEAM study, results showed that (1) during times conducive to accumulation of high outdoor VOC concentrations, substantial contributions to indoor levels can be made, and (2) in homes where there are no indoor sources of a VOC compound, the indoor concentration variation can be driven by outdoor VOC levels (Lioy et al. 1991).

4.3.2.2 Mass Balance Model Approach

For estimating air pollutant concentrations for indoor microenvironments, TRIM.Expo will include the option of using a mass balance modeling approach where sufficient data exist. In general terms, the mass balance model can be described as:

The change in indoor pollution concentration =
the pollutant entering from outside
+ the indoor generation of pollutant
— pollutant leaving the indoor microenvironment
— removal of the pollutant by an air cleaning device
— decay of the pollutant indoors.

Each term in the above conceptual model requires data inputs. Implicit in the above terms are data needs for other variables such as infiltration, air exchange rate, surface reactivity, building volume, and recirculation. Additionally, air exchange removal can be separated into fractions removed for unfiltered and filtered air, and similarly penetration of outdoor air can be separated into fractions for penetration of filtered and unfiltered air. Another factor which has a great influence on several of these variables is the type and use of air conditioning. One of the most ubiquitous sources of indoor air pollutants is smoking. This source type (when present) is responsible for elevated indoor concentrations of numerous air pollutants. Section 5.2.1 of this report describes in more detail the mass balance model that will be included in the initial inhalation prototype of TRIM.Expo.

McCurdy (1994) discusses the "indoor data factors and parameters" that were required inputs to the mass balance model used in pNEM/O_3. These factors, along with seasonal considerations, affect how much outdoor air pollution is estimated to come inside and how much indoor sources affect the indoor exposures. For the pNEM/O_3, values for most of the variables in its mass balance model are obtained by Monte Carlo sampling from empirical distributions of measured data. The variables include (McCurdy 1994):

- Probability of having open windows, given the type of air conditioning system found in the home and the outdoor temperature;
- Air exchange rate, which is also affected by the "window status";
- Residential surface-to-volume ratio, which is necessary to determine surface reactivity losses; and

- Emission rates from any indoor sources and the probability that the sources will be operating or not.

There is an ever increasing database for all of the factors mentioned above. For example, the Source Ranking Database provides data on indoor source emission factors (Johnston et al. 1996). In addition, the U.S. Census Bureau, as part of its American Housing Survey, routinely collects information on housing and building characteristics, including the use of air conditioning, methods of heating, square footage, and number of rooms. Researchers have become much more aware of the importance of seemingly minor factors such as whether a house's windows were open or shut when conducting studies of indoor and outdoor air pollutants. As a result, new studies are providing distributions for these important factors. Johnson et al. (1996a) provides a literature survey of recent studies for many of these factors. EPA will examine available databases such as the Source Ranking Database and American Housing Survey for relevant information on indoor sources and housing and building characteristics that can be used in TRIM.Expo.

4.3.2.3 Empirical Indoor/Outdoor Ratios Approach

The use of empirical indoor/outdoor relationships for estimating pollutant concentrations for indoor microenvironments is an approach that is often used when measured pollutant data or data needed for a mass balance model are lacking. This approach relies on observed relationships between outdoor concentrations and concurrent indoor or in-vehicle microenvironmental concentrations for selected pollutants. The Hazardous Air Pollutant Exposure Model (HAPEM4), a model similar to pNEM, uses this approach for estimating indoor and in-vehicle microenvironmental concentrations. The HAPEM4 uses a method of indoor/outdoor ratios called "microenvironmental (ME) factors" for determining the pollutant concentration in each indoor or in-vehicle microenvironment.

The EPA's OAQPS is currently collecting and analyzing data relevant to the development of ME factors for HAPs corresponding to those addressed in Section 112(k) of the Clean Air Act Amendments of 1990. Eventually, ME factors will be developed for all HAPs listed under Title III of the CAA. In addition to the traditional ME factor (also referred to as the penetration factor), data will be collected whenever possible for a separate factor relating the closeness of key sources to a microenvironment. Referred to as the proximity factor, this factor accounts for the higher concentrations usually expected when a receptor moves closer to a source. The resulting ME factors used in HAPEM4 are given by the expression:

$$C_{in}(i,k,t,cq) = \{[\gamma(k,cq)][C_{out}(i,t,cq)][\alpha(k,cq)]\} \tag{4-13}$$

where:

$C_{in}(i,k,t,cq)$	=	Average pollutant concentration in microenvironment k at exposure district i during time step t for calendar quarter cq.
$\gamma(k,cq)$	=	Penetration factor (relates outdoor concentration to indoor or in-vehicle microenvironmental concentration).

$C_{out}(i,t,cq)$	=	Ambient pollutant concentration taken at a fixed-site monitor or from a modeled value.
$\alpha(k,cq)$	=	Proximity factor (relates the closeness of key sources to a microenvironment).

Note that the ME factors typically do not vary by exposure district or from one time step to the next. However, they may be affected by calendar quarter (*i.e.*, by season).

4.3.3 ACTIVITY PATTERN DATA

Activity pattern data are used to determine the frequency and duration of exposure for specific groups within various microenvironments. As mentioned in Chapter 2, information on activity patterns are taken from measured data collected during demographic surveys of individuals' daily activities, the amount of time spent engaged in those activities, and the locations where the activities occur. Two common methods for collecting these data are through diary studies and activity recall studies. Diary studies involve a volunteer carrying a specially designed time-activity diary with them during their daily routine. They use the diary to record the start time of the activity, their location at the time, a description of the activity, the time the activity ended or changed to another one, and, sometimes, an estimate of their breathing rate. Diaries can be designed to obtain additional information for specific purposes or study requirements. In an activity recall study, respondents are asked to complete a questionnaire that details their activities from memory. The respondent is typically asked to recall his or her activities at the end of each day for the preceding 24-hour period. Data from this type of study are usually not as detailed as. However, activity recall studies can generally be conducted on larger populations than diary studies, since large numbers of respondents can be contacted by telephone.

In addition to recording the duration and location of a person's activities, important demographic information about the person is also then collected. The demographic information usually includes the person's age, gender, and ethnic group. Most activity pattern studies also try to collect information on other attributes of a respondent, such as highest level of education completed, number of people in their household, whether the person or anyone in their household is a smoker, employment status, and the number of hours spent outdoors. These are a sample of the possible items that might be requested on a questionnaire.

One of the largest databases for human activity pattern data is EPA's Comprehensive Human Activity Database (CHAD) (Glen et al. 1997). CHAD is comprised of nearly 17,000 person-days of activity pattern data. At present, 140 activities and 114 locations are included in CHAD. The data have been collected and organized from eight human activity pattern surveys. CHAD contains the sequential patterns of activities for each individual. Each activity has a corresponding location code so that the microenvironment of each activity is known. The activities in CHAD range from one minute to multiple hours in duration (activities longer than one hour are broken into segments and do not cross over from one clock hour to the next). The CHAD also provides an indicator of the rate of energy expenditure during a particular activity for each exposure event. This indicator is the metabolic equivalents or "METs" (see Section 6.1.5

for a description). In addition, CHAD includes an estimate of the body mass for each individual. This parameter is important for calculating uptake and dose (McCurdy 1999).

The TRIM.Expo module will have the ability to use the data in CHAD or, alternatively, use the data from a particular survey directly, providing the data are formatted properly. The CHAD will be updated periodically as additional data from new time/activity pattern surveys become available. In this way, a user has the two option mentioned above for using time/activity survey data in TRIM.Expo.

4.3.4 DEMOGRAPHIC AND AT-RISK POPULATION DATA

One of the purposes of TRIM.Expo is to perform analyses for subsets of the population that are particularly at risk to exposure to pollutants because of age or preexisting medical conditions. There are many sources of information detailing the demographic character of the population for the U.S. The originating source for most of this information is the Bureau of the Census (BOC), which compiles detailed demographic information about the U.S. population every ten years. The information is collected for the entire country at the census “tract” level or for the smaller census “block.” Census tracts are small, relatively permanent statistical subdivisions of a county. Census tracts usually include between 2,500 and 8,000 persons. Census tracts do not cross county boundaries. The spatial size of census tracts varies widely depending on the population density of the area. Census blocks are smaller than census tracts in areal extent.

The BOC collects data on numerous aspects of the demographic character of U.S. citizens, including national and state population trends and projections; geographical mobility; school enrollment; educational attainment; households and families; marital status and living arrangements; fertility; child care arrangements; child support; disability; health insurance; labor force and occupation; income and poverty; and characteristics of various ethnic and elderly populations. Much of this information can be useful for understanding the demographic patterns that put segments of the population at risk from exposures to environmental pollutants.

Although the census is a good source of information about the geographic, housing, business related, and demographic characteristics of the U.S. population, it is limited in the amount of information available about the general health status of the population. However, there are other sources of information available about the incidence of diseases and illnesses in the U.S. For example, the National Center for Health Statistics (NCHS) publishes data from its National Health Interview Survey (NHIS). The households selected to be interviewed each week in the NHIS are a probability sample representative of the target population. Data are collected annually from approximately 43,000 households including about 106,000 persons. Data collected includes household composition, sociodemographic characteristics, basic indicators of health status, and utilization of health care services. Other information sources published by NCHS include the National Health and Nutrition Examination Survey, Ambulatory Health Care Data, and the National Maternal and Infant Health Survey. These databases can be used to estimate the size of various at-risk population groups.