APPENDIX AVAILABLE ON REQUEST

Research Report 160

Personal and Ambient Exposures to Air Toxics in Camden, New Jersey

Paul J. Lioy et al.

Appendix H. Modeling Methods

[Note: Appendices Available on the Web appear in a different order than in the original Investigators' Report. HEI has not changed these documents. Appendices were relettered as follows:

Appendix H was originally Appendix VI

Correspondence may be addressed to: Dr. Paul J. Lioy, Environmental and Occupational Health Sciences Institute, Piscataway, New Jersey 08854

Although this document was produced with partial funding by the United States Environmental Protection Agency under Assistance Award CR–83234701 to the Health Effects Institute, it has not been subjected to the Agency's peer and administrative review and therefore may not necessarily reflect the views of the Agency, and no official endorsement by it should be inferred. The contents of this document also have not been reviewed by private party institutions, including those that support the Health Effects Institute; therefore, it may not reflect the views or policies of these parties, and no endorsement by them should be inferred.

This document was reviewed by the HEI Health Review Committee
but did not undergo the HEI scientific editing and production process.

Appendix VI. Modeling Methods

MENTOR links state-of-the art predictive models of environmental fate/transport with human exposure and dose estimation models. These models are coupled with up-to-date national, regional, and local databases of environmental, microenvironmental, biological, physiological, demographic, etc. parameters to characterize exposures/doses to environmental contaminants (Georgopoulos and Lioy 2006). Thus MENTOR is not a "model"; it is an evolving open computational toolbox, containing both "pre-existing" and new tools, intended to facilitate consistent multiscale source-to-dose modeling of exposures to multiple contaminants, for individuals and populations. For the IBEM application, the generalized 7-step approach has been developed in the MENTOR system (the details are described in Georgopoulos and Lioy 2006). It accounts for the processes determining exposures/doses from source-to-dose. It was used specifically to characterize personal exposures to three air toxics: Benzene, Toluene, and Formaldehyde. Seven steps comprise the IBEM approach (Georgopoulos and Lioy 2006) and this study has applied the firs 6 steps to characterize personal exposures. These are:

1. Estimation of background levels through:

(a) multivariate spatiotemporal analysis of monitor data, or

(b) emissions-based air quality modeling (with regional, grid-based models: Models-3/CMAQ [(Byun and Ching 1999)] and CAM-x [(Environ 2005)]

In this step, option (a) was used.

2. Estimation of local outdoor pollutant levels that characterize the ambient air of an administrative unit (such as a census tract) or a conveniently defined grid through

(a) spatiotemporal statistical analysis of monitor data

(b) subgrid "corrections" of multiscale model estimates, or

(c) application of a local scale air quality model such as ISCST3, AERMOD, etc.

In this step, option (c), applying both ISCST3 and AERMOD, was used.

3. Development of database of individual subjects attributes (residence and work location, housing characteristics, age, gender, race, income, etc.) through

(a) collection of study-specific information

(b) supplementing study-specific information with available, relevant local, regional and national information

In this step, option (a) was used.

4. Development of activity event (or exposure event) sequences for each individual in the study for the exposure period by

(a) using study-specific information

(b) supplementing study-specific information with other available data

(c) organizing time-activity database in format compatible with the Consolidated Human Activity Database (CHAD) [(Hubal et al. 2000)]

In this step, option (a), the time-location logs provided by the subjects, was used.

5. Estimation of levels and temporal profiles of pollutants in various microenvironments (streets, residences, offices, restaurants, vehicles, etc.) through one (or a combination) of the following methods:

(a) linear factors

(b) regression of observational data

(c) simple linear mass balance

(d) detailed (nonlinear) gas/aerosol chemistry models

(e) detailed combined chemistry and fluid dynamics models

In this step, option (a) was used.

6. Calculation of appropriate inhalation rates for the study subjects combining the physiological attributes of the study subjects and the activities pursued during the individual exposure events. In this study, the inhalation rates of the study subjects were not calculated for estimating the intakes. Instead, personal exposure was calculated as time-weighted average of estimated microenvironmental concentrations that each subject has experienced during the personal sampling period.

The following sections describe how the above steps of the generalized individual-based exposure modeling have been implemented for this study.

Estimation of Background Levels of Air Pollutants

For many toxic air pollutants, outdoor concentrations should include “background” attributable to long-range transport, unidentified emission sources, and natural emission sources. To estimate total ambient concentrations of air toxics, it is necessary to account for background concentrations not represented by atmospheric modeling of anthropogenic emissions. The background levels for two (benzene and formaldehyde) of the three selected air toxics were characterized by extracting the annual average background concentration estimates in Camden county, NJ from the 1999 NATA study [(USEPA 2006b)]. For benzene, the background concentration of 0.43 μg/m^3 was used. For formaldehyde, the background concentration of 0.87 μg/m^3 was used.

Estimation of Local Ambient Pollutant Levels

Atmospheric dispersion modeling using as inputs source emissions data and local meteorological conditions was conducted to calculate the 24-hour average ambient concentrations and were matched in space and time with the ambient measurements collected from the field study. Model receptors were defined as two ambient stationary monitors (WFS and CDS) and subjects' homes. The U.S. Environmental Protection Agency (EPA) has developed regulatory air dispersion models and modeling guidance, including recommended models whose performance has been tested against measurements (NARA 1999). Both of the ISCST3 and AERMOD dispersion models were used in this study, and their performance in predicting ambient concentrations of air toxics was tested for the WFS and CDS . The following sub-sections describe how the model inputs of sources emissions and meteorological data were prepared for the atmospheric dispersion modeling.

<u>Preprocessing of emission inventories (preparatory step 2a)</u>

The processed emission data for both Camden and Philadelphia counties are described in Section B.6.3.1 and presented in Table 7 and Figures 8 to 10. The study of Pratt et al. recommended treating mobile sources on major highways as line sources rather than area sources distributed at census tracts for better characterization of the impact of mobile on-road emissions on the nearby receptor location. Therefore, in addition to spatially allocate the county level mobile on-road emissions into census tracts (shown in Figures 8 to 10) we improved the mobile on-road emission inputs by allocation to roadway links. Sensitivity simulations using the ISCST3 model were carried out by applying the two different mobile on-road emission inputs to examine their impact on the predictions of ambient concentrations.

The limitation of the county level emissions estimates in the 2002 NEI is that these data may under-estimate the sources emissions due to localized factors in "hot-spots". For example, the county-level mobile on-road emissions of the 2002 NEI were estimated by the products of emission factors (in grams or milligrams per mile) and vehicle activity levels (e.g., vehicle miles traveled). These emission factors represent long-term county level vehicle population averages and vehicle activity data. Although these mobile source emissions were apportioned to census tracts, the emissions estimates may not reflect local scale conditions of heavy traffics, such as heavy truck traffic passing through WFS as reported by the NJDEP (2005).

Preprocessing of local meteorology information (preparatory step 2b) as presented in Section B.6.3.1.

Microenvironmental and Personal Exposure Modeling

The dispersion model prediction of outdoor concentrations for the three air toxics were used as the ambient inputs to derive profiles of microenvironmental concentrations that each subject would have experienced during each of the monitoring periods. Personal exposure concentrations were then calculated using IBEM as the weighted average microenvironmental concentrations using the durations of times spent in the microenvironments as weights for each subject. The ambient measurements collected at the two central-site monitors (WFS and CDS) were used as a second option for ambient inputs to calculate the microenvironmental and personal exposure concentrations.

Information on the duration of time spent in the microenvironments was extracted from the time-activity diary (Appendix III). Specifically, the subject-specific time-activity diaries collected along with the personal measurements in the field study provided information about where the subjects spent their time among five microenvironments (home, office/school, other indoors, outdoor, and in-vehicle) in a sequence of hourly exposure events during the 24-hour personal monitoring period. These diaries provided the critical information on where and when the exposures occurred and these were used in estimating the personal exposures for each of the subjects, and are not normally used in personal exposure applications.

A database for time-activity information based on these subject-specific diaries was developed as input variables in a format compatible with the default database, CHAD. In developing this time-activity database, a practical issue of treatment of missing records for activity events was considered, since these diaries were collected based on the subjects' recall and the individual might not remember all the detailed information. The raw data of the time-activity diaries were screened first to exclude those diaries with severe number of missing records. The following rules were used to impute the missing records.

- (a) If the subject's diary has one hour of missing record, combine the information from adjacent previous and later hours as the imputed record.
- (b) If the subject's diary has two continuous hours of missing records, use the record from adjacent previous hour for the 1st missing hour and the record from the adjacent later hour for the 2nd missing hour.

- (c) If the subject's diary has three continuous hours of missing records, the 1st and 3rd missing hours follow the rule (b) and the 2nd missing hour follows the rule (a) to impute the missing records.

Further, 34 subjects carried the GeoLogger device to track their movements during the personal sampling periods. By cross-checking the Geologger data with the time-location logs provided by these subjects, the quality of the time-activity data could be better assessed (see Appendix V for details).

Microenvironmental Modeling Approach

The microenvironmental module of the MENTOR system was used to derive temporal profiles of five microenvironmental (home, office/school, other indoors, outdoor, and in-vehicle) concentrations for the three selected air toxics based on ambient concentration estimates obtained from step 2. Different modeling algorithms options for calculating microenvironmental concentrations are available in the MENTOR system as described in the generalized 7-step approach above. In this study, the approach of linear factors was used to estimate the microenvironmental concentrations based on the following equation:

$$ME(m,r,t) = ADD(m) + [PROX(m)][PEN(m)][AMB(r,t)]$$

where:

- *ME(m,r,t)*: concentration of microenvironment *m* in receptor location *r* at time *t*,
- *ADD(m)*: additive factor for microenvironment *m*,
- *PROX(m)*: proximity factor for microenvironment *m*,
- *PEN(m)*: penetration factor for microenvironment *m*, and
- *AMB(r, t)*: ambient concentration in receptor location *r* at time *t*.

The additive factor accounts for the contribution of emissions sources from indoors. This term was set to zero, since the focus of this analysis was to estimate the contribution from ambient sources of air toxics to personal exposures. The proximity factor (*PROX*) accounts for the relationship between the outdoor concentration in the vicinity of the microenvironment and the ambient concentration at the receptor location represented by *AMB(r,t)*. This factor was set to 1 based on the fact that the central-site monitors were quite close to the receptor locations of the subjects' residences. The penetration factor (*PEN*) represents the ratio of the microenvironmental concentration to the ambient concentration in the immediate vicinity of the microenvironment, when the microenvironment contains no indoor sources. Based on the compilation of extensive literature reviews for the Indoor/Outdoor (I/O) ratios at different microenvironments, *PEN* factors for various air toxics have been developed as part of the 1999 National Air Toxics Assessment (NATA) study [(USEPA 2006a)]. The *PEN* factors for the three selected air toxics (benzene, toluene, and formaldehyde) were extracted from the 1999 NATA database to calculate the microenvironmental concentrations. For testing the impact of using different ambient concentration estimates on the predicted personal exposures, the following options were used one-by-one as the ambient inputs to calculate microenvironmental concentrations: ISCST3 calculations, AERMOD calculations, and the ambient measurements.

Personal Exposure Modeling Approach

Personal exposure concentrations were estimated by combining the information from activity diaries with the modeled microenvironmental concentrations. Specifically, the time and location recorded for each exposure event of the time-activity diary were used to extract the corresponding microenvironmental concentrations that each subject experienced during the personal monitoring period. The time-series of hourly personal exposure concentrations was then generated for each subject, when the atmospheric dispersion modeling results were used as ambient inputs. The average of these hourly personal exposure concentrations was then calculated for the comparison with the corresponding 24-hour integrated personal air measurement for each subject. When an ambient measurement was used as the ambient input, the time-weighted average of personal exposure concentration was calculated instead of the hourly time-series, since the ambient measurement was a 24-hour integrated sample.

For some exposure events listed as part of the time-activity diaries, multiple locations of microenvironments were recorded for a single event, but no further information collected about how the subject spent his/her time at these locations during the one hour exposure event. In such a case, the assumption was made that the subject spent his/her time evenly among the multiple microenvironments recorded in this hour, and the personal exposure was calculated by averaging