ISSUES AND CHALLENGES IN MODELING CHILDREN'S LONGITUDINAL EXPOSURES: AN OZONE CASE STUDY

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ABSTRACT

Modeling children's exposures is a complicated, data-intensive process. Modeling longitudinal exposures, which are important for regulatory decision making, especially for most air toxics, adds another level of complexity and data requirements. Because it is difficult to model inter- and intra- personal variability for exposure model inputs, there is potential for inaccurate estimation of upper percentiles of longitudinal exposure distributions. In order to develop a scientifically sound exposure prediction model, we need to resolve how to do the following: (1) obtain longitudinal data needs for time activity and pollutant measurements; (2) separate intra- and inter- person variability of model inputs; (3) link inputs from different data sources and fit those data as inputs for the model, which will preserve its variance-covariance structure; and (4) use cross-sectional data to simulate longitudinal data, which is difficult and expensive to collect.

In this presentation, we address these issues by applying both an existing and a new technique for estimating personal ozone exposures of school-age children living in two California communities. The first modeling analysis employed commonly used methods for estimating exposures using a microenvironmental exposure model that used independent distributions in simulations, which were fit to observed inputs for the model. In the new modeling methodology, various variance components derived from the underlying data were put back into model, so that proper variance-covariance relationships in model inputs were maintained. Contribution of intra-personal, inter-personal, seasonal, and area's variances predicted by the new model, were: 38%, 19%, 39% and 4%, which were quite close to those derived from the original data while intra-personal variance is 91% for the old method without decomposition of the variance. The standard deviation and 99th percentile of overall personal ozone exposures from the model with the new method and the old method without decomposition of variance of intra, inter personal and other factors, were: 12 ppb, 53 ppb and 21 ppb, 89 ppb, respectively, and in comparison to 12 ppb, 52 ppb for the observed personal ozone data. Results show that this method not only can keep variance-covariance structures of inputs and output in a simulation, but also can accurately predict high percentiles of longitudinal exposures that are important for regulatory evaluations.

INTRODUCTION

General Modeling Questions

- How can we best determine children's exposures to various environmental agents by different life stages?
- Which locations, sources, media, routes and pathways contribute greatest to exposures of interest?
- What activities and behaviors influence the pollutant contact rates, exposures, uptake and dose?
- What are the measures of exposures of health relevance (e.g., duration, intensity, timing, frequency)?
- How do exposure and physical factors vary by age, gender, susceptibility, personal habits (e.g., cooking and cleaning exposures, second hand smoke), housing type, consumer product usage?
- How do subject-specific longitudinal correlations of personal exposures with outdoor concentrations vary?
- How are microenvironmental concentrations of $PM_{2.5}$, ozone, air toxics correlated?
  - Ambient central site vs. outdoor
  - Indoor residential vs. outdoor
  - Personal vs. outdoor

Challenges

- Lack of longitudinal spatial and temporal concentration data
- Lack of longitudinal activity data
- How to simulate height and weight, activity patterns and breathing rates for children as they grow older?
- How to use cross-sectional data to simulate longitudinal data?
- How to separate intra- and inter- person variability of model inputs?
- How to preserve variance-covariance structure of inputs when combining different data sources in exposure models (see Ozone Case Study)?

ISSUES

Pollutant Sources of Concern

- Indoor or outdoor combustion sources
- Nearby ETS and PM generating activities
- Ambient fine and ultrafine PM
- VOCs from proximity to mobile sources/refueling/attached garages
- Air toxics from consumer products and hobbies
- Indoor and outdoor aeroallergens
- High outdoor ozone/photochemical smog

Concentration-Related

- What are the relevant microenvironments (see Figure 1)
- Do children spend more time indoors (schools, daycare) or in other microenvironments than the adults in the population (see Figure 2)?
- Do children engage in fewer pollution generating activities than the other age groups?
- Do personal exposures of children correlate well with outdoor

Figure 1. Relevant Indoor Microenvironments for Children

Figure 2. Relevant Outdoor/In-Vehicle Microenvironments for Children

Activity-Related

- Where do children spend their time with respect to relevant pollutant-containing microenvironments (see Figure 3 for an example of a time-activity diary)?
- Do children spend more time indoors (schools, daycare) or in other special microenvironments than the rest of the population?
- Do children engage in fewer pollution generating activities than other cohorts?
- Are time-activity profiles of children appreciably different than those for the general population?
- Do children engage in different types of personal activities which generate elevated indoor or personal exposures to PM, combustion gases and air toxics?
- How do children's exposures differ as a function of childhood life stages?

Fig 3. Example Human Activity Diary from EPA's Consolidated Human Activities Database (CHAD) (http://www.epa.gov/chadnet1/)

Age-Grouping for Children

- EPA guidance on age grouping is supported by an underlying scientific rationale (Figure 4)
- Use in exposure and risk assessments for consistency
- Foundation for future exposure factors and/or monitoring data generation/analysis
- U.S. EPA (2005). Guidance on selecting age groups for monitoring and assessing childhood exposures to environmental contaminants. Risk Assessment Forum, Office of Research and Development, Washington, D.C. EPA/630/P-03/003F. http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=14658

Fig. 4. EPA Guidance on Age Groups for Exposure Assessments

	Infancy	Young toddler	Older toddler	Preschool	Adolescence	High School/College
	birth to < 1 month	1 to < 3 months	3 to < 6 months	6 to < 12 months	1 to < 2 years	2 to < 3 years	3 to < 6 years	6 to < 11 years	11 to < 16 years	16 to < 21 years

METHODS

Model Types

- Empirical models
  - Developed using empirical data from personal monitoring studies
  - Example: Regression equations that explain measured exposures
- Deterministic/mechanistic models
  - Based on known or assumed physical relationships
  - Example: Air quality models, pharmacokinetic models
- Stochastic/mechanistic models
  - Input data are distributions, not single value
  - Input distributions characterize variability/uncertainty in the data
  - Use Monte Carlo or other random sampling techniques
  - Produces output distributions (variability/uncertainty)

$$E = \sum_i E_i = \frac{1}{T}\left(\sum_i \overline{C}_i t_i\right)$$

Modeling Elements

- Identify cohorts and microenvironments of concern
- Collect available time-activity data
  - Locations spent time in and the activities performed while in a location
  - Age, gender, region, etc.
- Collect available microenvironmental measurements
  - Concentrations outdoors, indoors, in-vehicle
- Estimate physical factors
  - Source use and emissions
  - Penetration, Infiltration, re-suspension, volatilization, decay Estimate exposure factors
  - Contact/transfer/uptake/PBPK rates or parameters
- Apply data and algorithms using a selected modeling structure to predict exposure distributions (see Figure 5 for $PM_{2.5}$ and Figure 6 for benzene exposures generated by the EPA's SHEDS model)
- Compare estimates to available personal exposure measurements

Figure 5. Distribution of Daily-average Total $PM_{2.5}$ Exposure and Uncertainty for Selected Percentiles in Philadelphia, PA Predicted by the SHEDS-PM Model
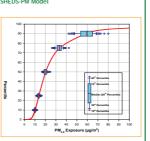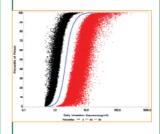

Figure 6. Daily Inhalation Exposures to Benzene in Houston, Texas predicted by the SHEDS-Air-Toxics Model

OZONE CASE STUDY

Approach

- Extend an earlier analysis conducted by Xue et al. 2005 by applying both an existing and a new technique for estimating personal ozone exposures of school-age children living in two California communities
- The first modeling analysis employed commonly used methods for estimating exposures using a microenvironmental exposure model that used independent distributions in simulations, fit to observed indoor, outdoor and time-activity data
- In the new modeling methodology, different variance components derived from the underlying data were put back into the model, so that proper variance-covariance relationships in model inputs were maintained: $\sigma^2_{total} = \sigma^2_{intra-person} + \sigma^2_{inter-person} + \sigma^2_{season} + \sigma^2_{area}$
- SAS mixed effects model procedure was used to decompose the major variance components of each of the ozone and time activity measures

Results

- Intra-personal, inter-personal, seasonal, and area related variances predicted by the new model were close to those derived from the original data, while intra-personal variance was overly inflated by the basic method which did not consider proper decomposition of the variance (Table 1)
- New exposure simulation method successfully retains the variance-covariance structure of different inputs and outputs, and can accurately predict both the annual average and the high percentiles of longitudinal exposures that are important for scientific and regulatory evaluations (Figures 7 and 8)

Table 1. Percent of Variance Explained by Intra-personal, Inter-personal, Season and Area Terms for Personal Ozone and Outdoor Time

variables	Variance decomposition (%)			
	intra	inter	season	area
observed personal ozone concentration	41.8%	13.3%	44.0%	0.8%
predicted personal ozone with observed data	32.6%	10.6%	50.2%	6.7%
predicted personal ozone*	91.3%	8.6%	0.1%	0.0%
predicted personal ozone with simulated inputs**	37.7%	18.7%	39.3%	4.3%
actual outdoor time near home	59.8%	33.4%	6.8%	0.0%

* Simulations without the decomposition of variances

** Simulations with decomposition of major variance terms

Figure 7. Measured and Modeled Annual Average Personal Ozone

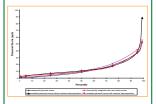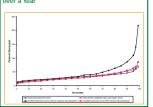#### Figure 8. Distributions of 95th Percentile Values of 7-Day Average Personal Ozone for each child over a Year

DISCUSSION

- It is important to model exposures of children by critical life-stages that represent both the developmental and the likely exposure-related changes over the first 6 years of life
- Children are exposed to different sources and concentrations of pollutants in various indoor, outdoor and commuting environments
- Additional data on physical, microenvironmental and exposure factors could improve current exposure predictions
- For modeling long-term exposures to air pollutants, age-specific longitudinal time-activity data and information on key determinants and components (e.g., intra- and inter-personal factors) of the variance of personal exposures are needed
- Probabilistic exposure simulation modeling with decomposition of variance terms is a promising approach that addresses these issues
- A case study based on data from Southern California, showed that by proper apportionment of the variance-covariance relationships in model inputs, it is possible to accurately predict the central values and the high percentiles of longitudinal personal ozone exposures of children

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