Diagnostic Evaluation and Refinement of Procedures for Modeling Exposures to VOCs

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This project brought together a diverse team of model developers and field exposure scientists from academia and consulting as well as collaborators (non-funded) from U.S. EPA's Office of Research and Development and Office of Air Quality Planning and Standards. Team members worked jointly to evaluate and improve modeling methods for assessing human exposures to mixtures of volatile organic compounds (VOCs). The research pursued included performing comparative evaluations of algorithms and methods used in state-of-the-science comprehensive exposure modeling systems, specifically the Hazardous Air Pollutant Exposure Model (HAPEM), Air Pollution Exposure Model (APEX) (the inhalation exposure component of TRIM.expo), the Total Risk Integrated Methodology (TRIM) system, and the Modeling Environment for Total Risk studies (MENTOR). These models have been used in various recent comprehensive modeling studies, including the 1996 and 1999 National Air Toxics Assessments (NATA) and the 1999 Philadelphia source-to-dose assessments for photochemical pollutants and particulate matter (PM) performed by the project team. As part of the project, the above models were evaluated for both a population-based exposure modeling approach, studying the sample population of the National Human Exposure Assessment Survey (NHEXAS) – Region V, and an individual-based modeling approach, focusing on the three sample populations (Elizabeth, NJ; Los Angeles, CA; Houston, TX) of the Relation among Indoor, Outdoor, and Personal Air (RIOPA) study. Outcomes of the study included as deliverables both modeling guidelines and user-oriented software tools that can help improve future local, regional, and national assessments of human exposures to air toxics and quantify the relative contributions of VOCs originating from both outdoor and indoor sources.

Specifically, the project accomplishments include comparative evaluation of various comprehensive exposure modeling systems, development of a multi-chemical exposure modeling system for modeling population exposures, development of an individual-based exposure modeling system for VOCs, and application of these systems to study individual and population exposures to reactive and non-reactive organics. The Database of Indoor Microenvironmental Emissions (DIME) was developed for indoor microenvironmental emissions of benzene, formaldehyde, trichloroethylene (TCE), and perchloroethylene (PERC). Refinements were also made to modules for simulating individual exposures to VOCs using local scale air quality models (Industrial Source Complex Short Term (ISCST3) model and AERMOD) with MENTOR-1A (i.e., MENTOR in a one atmosphere setting) for "hot-spot" areas.

New MENTOR-1A modules were developed for studying population exposures to multiple, co-occurring VOCs. These modules are amenable to long-term (e.g., year-long) exposure calculations. MENTOR-1A was applied to assess the impacts of commuting patterns, roadway effects, indoor sources of air toxics, and complex atmospheric chemistry on population exposure assessments. Case studies focused on indoor sources of benzene (smoking, garages, and emissions from wood parquet), and outdoor contributions of formaldehyde. The simulation results highlighted the need for accurate characterization of distributions of the indoor source emissions. The results from a year-long simulation were compared with results from an existing exposure modeling system (APEX) that was used to conduct an analysis for the same general population as that modeled by MENTOR-1A. The comparison allowed for a characterization of the "model uncertainty" as reflected in the distributions of population exposures. Additionally, new MENTOR-1A components were developed in order to facilitate the use of complex exposure models by non-specialists, while reducing the time required for simulation using "pre-computed" modeling.

Simulations were conducted to assess individual exposures to benzene and toluene for approximately 108 subjects of the Air Toxics-Camden field study in a "hot-spot" area of Camden, NJ, during 2004-2006. The simulation results were compared with corresponding neighborhood and personal exposure measurements. The modeled ambient concentrations of benzene and toluene were generally in agreement with the neighborhood measurements within a factor of two, but were underestimated at the high-end percentiles. The percent contributions of personal exposures to the two VOCs resulting from ambient sources were also estimated by using local ambient measurements and subject-specific time-activity pattern data collected from the field study. Furthermore, comparative evaluations of local-scale air quality modeling methods were performed using Computational Fluid Dynamics models, street canyon models, and dispersion models.

During 2008, manuscripts summarizing and analyzing the results and findings of the project were prepared and submitted. One manuscript, focusing on the application of the individual-based exposure modeling was accepted for publication and is in press, while two manuscripts are in the final stages of review and ready for submission. Additionally, one manuscript is in preparation. One book chapter on exposure modeling, containing findings from the project has been accepted.

Implications: Model evaluations and refinements pursued during the project can improve future modeling tasks in support of decision-making processes as they help identify the most appropriate algorithms and parameterizations for specific applications. This approach reduces and quantifies uncertainties associated with various modeling estimates. The outcomes of the project have resulted in improvement of the overall understanding of microenvironmental exposures to VOCs, and of the factors which influence them.

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Presentations:

Georgopoulos, P.G., Isukapalli, S., Wang, S.W., Lahoti, N., Yang, Y.C., Burke, J., Özkaynak, H., Ching, J., and Pierce, T. (2004). Source-to-dose modeling of long-term population exposures to co-occurring reactive and inert air pollutants. Presentation at ISEA 14th Annual Conference – Exploring Emerging Technologies for Exposure Assessment, Philadelphia, PA.

Georgopoulos, P.G., Isukapalli, S., Wang, S.W., Yang, Y.C., Zartarian, V., Xue, J., and Özkaynak, H. (2004). Modeling cumulative and aggregate exposures of co-occurring multimedia contaminants in a probabilistic source-to-dose framework. Presentation at ISEA 14th Annual Conference – Exploring Emerging Technologies for Exposure Assessment, Philadelphia, PA.

Georgopoulos, P.G. (2004). The modeling environment for Total Risk Studies (MENTOR). Toxicokinetic models and data for chlorinated VOCs: A Bayesian optimization approach. Presentation at USEPA National Center for Exposure Assessment, Washington, DC.

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Isukapalli, S., Wang, S.W., Georgopoulos, P.G., Pierce, T., and Ching, J. (2005). A modular system for source-to-dose exposure modeling of co-occurring air pollutants: recent developments and computational implementation. Presentation at the 4th Annual CMAS Models-3 Users'Conference, Chapel Hill, NC.

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Isukapalli, S., Langstaff, J., Ching, J., Luecken, D., and Georgopoulos, P. Comparative evaluation of approaches for modeling inhalation exposures for populations: Case study with the MENTOR and APEX systems. (In preparation).

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