8.6 NEIGHBORHOOD SCALE MODELING OF $PM_{2.5}$ AND AIR TOXICS CONCENTRATION DISTRIBUTIONS TO DRIVE HUMAN EXPOSURE MODELS

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1. INTRODUCTION

Air quality (AQ) simulation models provide a basis for implementing the National Ambient Air Quality Standards (NAAQS) and are a tool for performing risk-based assessments and for developing environmental management strategies. Fine particulate matter ($PM_{2.5}$), its constituents and size and number distribution, as well as airborne toxic pollutants ("air toxics") have characteristically different degrees of spatial and temporal variability especially in urban areas and in different geographical-climatic regimes. In this study, we explore the specific role of AQ models as a means to drive human exposure models (Burke et al. 2001) and to address situations in which pollutants exhibit high spatial and temporal variability. We seek a capability to capture the resolved-scale concentration fields and to provide measures of sub-grid-scale variability in concentration distributions that impact human exposures. This modeling approach is meant to enhance and complement the more limited data from central site monitoring networks to provide the concentration fields at high temporal and spatial resolutions. By providing further information on concentration variability at sub-grid scales, we complete the requirements needed for exposure assessments. The various elements of this modeling approach and some of their specific modeling issues are described below.

2. APPROACHES AND SCOPE

Our goal is to simulate the chemical and physical attributes of $PM_{2.5}$ and air toxics such that the output fields can be used to address both the traditional air quality management needs and to perform modeling of human exposure to various air pollutants. For this effort, we begin with the Models-3/Community Multiscale Air Quality (CMAQ) modeling system. CMAQ has a "one-atmosphere", multiple-pollutant capability (Byun and Ching, 1999) and thus is well suited to handle the photochemistry and other important atmospheric processes that impact the fate and transport of air pollutants. We anticipate that different pollutants will have characteristic spatial scales that the CMAQ multiscale capability will capture. Strategies to reduce human exposures can then be developed using emission projections.

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Next, human population exposure assessments will require an urban modeling emphasis. CMAQ and its pre-processing models will be modified with appropriate methodologies to handle urban morphological features and vegetation coverage. The added complexity of dispersion of pollution sources distributed within urban areas introduces additional complexity to modeling the concentration variability, an important consideration for exposure assessments. Finally, linkage to human exposure models will require information and modeling of human activity of the population and of pollution exchange between ambient and the various microenvironments (Ching et al. 2000). Modeling linkages to human exposure modeling will not be discussed here.

3. IMPLEMENTATION

3.1 *Resolved-Scale Modeling*

The simulation of the complex dispersion and transport at the neighborhood scales (~1 km horizontal grid spacing) is an important first step. We developed and implemented an urban canopy parameterization for the Pennsylvania State University, National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5) (Grell et al. 1994), which is used to provide meteorological fields for the chemistry-transport model in CMAQ. The urban canopy parameterization (Lacser and Otte, 2002) combines urban building morphologies with urban land use categories to produce meteorological fields that include the heterogeneous effects of the urban areas at that scale. This urban canopy parameterization is based on the drag approach (e.g., Brown 2000), and it is applied to grid cells in MM5 that have a non-zero fraction of urban land use. The horizontal components of the momentum equations and the turbulent kinetic energy (TKE) equation were modified to account for the area average effect of the sub-grid urban elements. The parameterizations produced significant differences in the mean and turbulent fields within the urban canopy, especially in areas characterized by high density of tall buildings. MM5 with the urban canopy parameterization simulated vertical profiles of wind speed and TKE that were highly consistent with results from wind tunnel studies. These results illustrate the importance of accounting for the urban morphological structures in modeling the flow in urban areas. It provides a basis for more accurately resolving the magnitude and spatial details of the modeled air quality fields, especially for pollutant

species that may have fine spatial gradients that are important for human exposure assessment.

3.2 *Sub-Grid-Scale Modeling*

A property of CMAQ (and most such grid models) is that the local, near-source concentration distributions due to dispersion of point, line, and area sources are not explicitly treated; rather, emissions from such sources are immediately dispersed throughout the grid volume. Thus, near-source concentrations will be higher than from the resolved-scale predictions, and consequently, exposure assessments will significantly underestimate the potential levels of human exposures in the near source areas. The design problem is to seek a model resolution that assures the inclusion of the important contributing atmospheric processes and also provides a means for estimating the near-source concentration distributions. For practical considerations, we address the latter requirement by developing concentration probability distribution functions, PDFs, for the sub-grid-scale concentration distributions. This system of resolved-scale and sub-grid-scale concentration distributions provides a more robust set of modeling outputs for human population assessments. We identify and propose methodologies for handling two contributing sources of this variability, including: (1) dispersion of point and area sources from street canyon flows using a combination of computational fluid dynamics and wind tunnel modeling techniques, and (2) direct coupling between turbulent motions and reactive pollutants when chemical reaction time scales are on the order of the turbulent eddy time scale (Herwehe 2000). In the latter case, a coupled large-eddy simulation photochemical model (LESchem) (Herwehe 2000) is used to address sub-grid-scale variability for pollutants with different chemical reactivity rates and turbulent transport time scales. Using this modeling approach, the chemistry and turbulent transport fields are solved as a coupled system, which allows bi-directional feedback between the chemistry and dynamics during the simulation.

4. RESULTS

Preliminary results for a case study for Philadelphia indicate that the extent of the resolved-scale spatial variability varies with each pollutant species, and the grid-resolved variability does not necessarily increase monotonically with increased grid resolution (Ching et al. 2000). This means that the grid resolution selected for use in exposure modeling may need to be ascertained by numerical experiments.

Analysis of the modeled time series of the hourly mean and standard deviation of $PM_{2.5}$ and the number density of particles in the Aitken nuclei mode shows large differences in the diurnal trend, as well as the degree and characteristics of spatial variability between these two parameters that show a sensitivity response to model grid size. Both the number and mass of the Aitken mode particles (including the ultra-fine particles) are believed to contribute to health risk.

Results to date for the sub-grid modeling focus on the turbulence-induced concentration fluctuations. Results indicate a wide range of sub-grid chemical variability dependent on pollutant species (e.g., large variability for formaldehyde and acetaldehyde; relatively small variability for carbon monoxide) at the surface as well as aloft in the mixed layer due to the degree of photochemical reactivity in atmospheric mixtures and various trace species chemical lifetimes.

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