Modeling Tools

An Overview of the Use of Air Quality Modeling In Support of Air Toxics Programs

Al Cimerelli and Jim Smith, EPA Region III
Modeling Tools

Part I:
Emissions Modeling and the Importance of Air Quality Modeling in Air Toxics
Jim Smith

Part II:
The Use of Air Quality Modeling In Support of Air Toxics Programs
Al Cimorelli
Purpose

- To outline what modeling work is being done for Philadelphia project.
- To describe how this work has changed our perception of the role that modeling must play in air toxics.
- To describe the use of EMS-HAPS for emissions pre-processing.
Initial modeling-related Goals of the Philadelphia Study

- To gain a more detailed, up-to-date picture of the health risks Philadelphia residents face from exposure to air toxics by:
  - Refining ’96 NATA risk estimates
  - Estimating present day risk (1999 inventory and 2010 projections)
- To better target efforts to reduce these health risks through culpability analysis.
- To develop internal capabilities for modeling air toxics
The Modelling Study in Philadelphia Includes the Following Pollutants

- Acetaldehyde
- Acrolein
- 1,3 butadiene
- Benzene
- Chromium
- Diesel PM
- Ethylene-Dichloride
- Formaldehyde
- POM
Modelling Grid & Urban/Rural Land Use

ISCST3 Urban (gray) and Rural (white) 1x1km Domain – Commercial/Industrial – threshold=25th percentile
modeling Work: Division of Labor

Consultant

- Extracted point, non-point and non-road inventories for grid from NTI
- Developed link-based mobile inventory
- Ran EMS-HAP

Region III

- Refined point inventory
- Reproduced EMS-HAP runs
- Ran ISC
- Ran HAPEM
- Analyzed results
Work Completed

- 1996 Inventory: Modeled the nine pollutants for 1990 population centroids and three 500 meter fine grids. (repeated runs when it was found that airport emissions were incorrectly located)

- 1999 Inventory: Modeled the nine pollutants for population centroids and three 500 meter fine grids. (ran with 1999 met data)
Example of Modelling Results: Benzene
Why Modelling is More Critical for Air Toxics

1. It is impractical to use *monitoring* to determine prevailing ambient levels of air toxics.
   - The number of air toxics to be monitored is large
   - Ambient levels of air toxics are highly localized

2. Decision-making for air toxics depends on *Risk* (lacking ambient air quality standards for all pollutants) and determining *Risk* requires modelling.
The Basic Tools for modeling Air Toxics

- The emissions processor (EMS-HAP)
- The Air Quality Model (ISC-ST3)
- The Exposure Model (HAPEM)
The Air Toxics Modeling Process

- Point emissions file
- Non-point emissions file
- Non-road emissions file
- Mobile emissions file

EMS-HAP (Emissions Processor) → HAPEM (Risk Model)

ISCST3 (Dispersion Model) → ANALYSIS)
The Focus Here: EMS-HAP

- Uses SAS Programming language (version 8)
- Inventory can be extracted from national inventory for selected grid and provided as SAS data file
- Designed for UNIX but can be adapted for PC
- Processes point, non-point, non-road and on-road emissions
- Cannot run MOBILE6 but can use link-based MOBILE6 generated emissions
- Prepares input files for either ASPEN or ISCST3
- Version 2 for 1996 NATA inventory; Version 3 for 1999 NEI and later (user’s guide for V3 still in draft form).
County-to-Point processing: extract certain county level sources and allocate to known locations

QA Locations & Stack Parameters

Model specific parameters

Selection, Partitioning and Grouping of Pollutants with optional source-based speciation

Spatially Allocate non-point & mobile source emissions

Temporally Allocate Emissions

Assign Source Groupings

Project Emissions

Format & Output Air Dispersion Model-Ready Emission-Related Inputs

Functions of EMS-HAP
Gridded versus non-gridded Emissions

- Point: non-gridded
- Airports: non-gridded is recommended
- Non-point: gridded
- Non-road: gridded
- On-road: non-gridded (link-based) is recommended
Spatial Allocation of County-level Emissions

Concept: use surrogates to allocate county level emissions for county-level sources

e.g., use population data to allocate consumer product emissions

This Grid cell gets 3/20 of Orange county’s consumer product emissions
Grouping Metal Compounds for Toxics Modeling in EMS-HAP

The HAP table groups, partitions and selects pollutants.

Example: Arsenic Coarse and Fine Pollutant Groups

<table>
<thead>
<tr>
<th>Name of Species</th>
<th>Description of HAP</th>
<th>Inventory pollutant code</th>
<th>Reactivity</th>
<th>KEEP</th>
<th>HAP CODE</th>
<th>Factor</th>
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<tbody>
<tr>
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<tr>
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<td>y</td>
<td>48</td>
<td>.41</td>
</tr>
<tr>
<td>Arsenic &amp; compounds</td>
<td>Arsenic cmpds coarse</td>
<td>601</td>
<td>3</td>
<td>y</td>
<td>48</td>
<td>.41</td>
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<td>48</td>
<td>.59</td>
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</tbody>
</table>
Speciating Chromium Compounds for Toxics Modeling in EMS-HAP V3

Specific HAP table can speciate using category specific data

Sample records in file supplied with EMS-HAP V3

<table>
<thead>
<tr>
<th>Speciated HAP</th>
<th>CAS</th>
<th>OldS1</th>
<th>NewS1</th>
<th>OldS2</th>
<th>OldS3</th>
<th>NewS3</th>
<th>SPECFX</th>
<th>MACT</th>
<th>SCC</th>
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</table>
Running EMS-HAP

- Multiple programs, run in sequence for each section of the inventory: point, non-point, non-road and on-road (airport emissions modeled at specific locations rather than gridded run separately).
- Each program is run using a batch file containing file names, directories and settings.
Resources required for EMS-HAP

- A SAS license is required
- It does require an initial investment of time to become familiar with SAS, set it up for a given grid and emission inventory
- But once the initial learning curve is over, it is relatively easy to use and uses little computer time
Why Your Agency Should Consider Using EMS-HAP

- Air Toxics Modeling is crucial for:
  - Understanding an area’s air toxics problems
  - Calculating risk
  - Proper placement of air toxic monitors
  - Setting priorities for enforcement and other decisions regarding air toxics

- EMS-HAP is *not* resource intensive
  - One person can run EMS-HAP and ISCST3