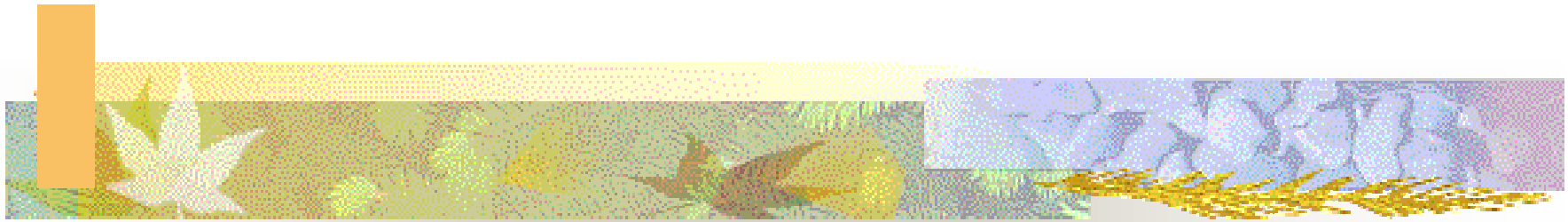
Modeling Tools

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



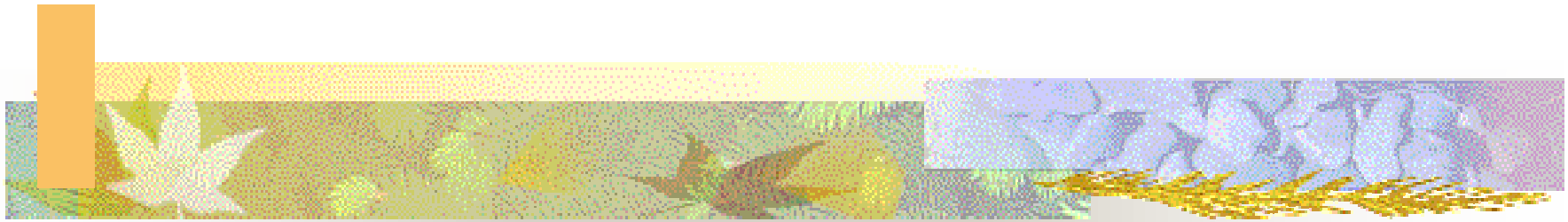
Al Cimerelli and Jim Smith, EPA Region III

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.

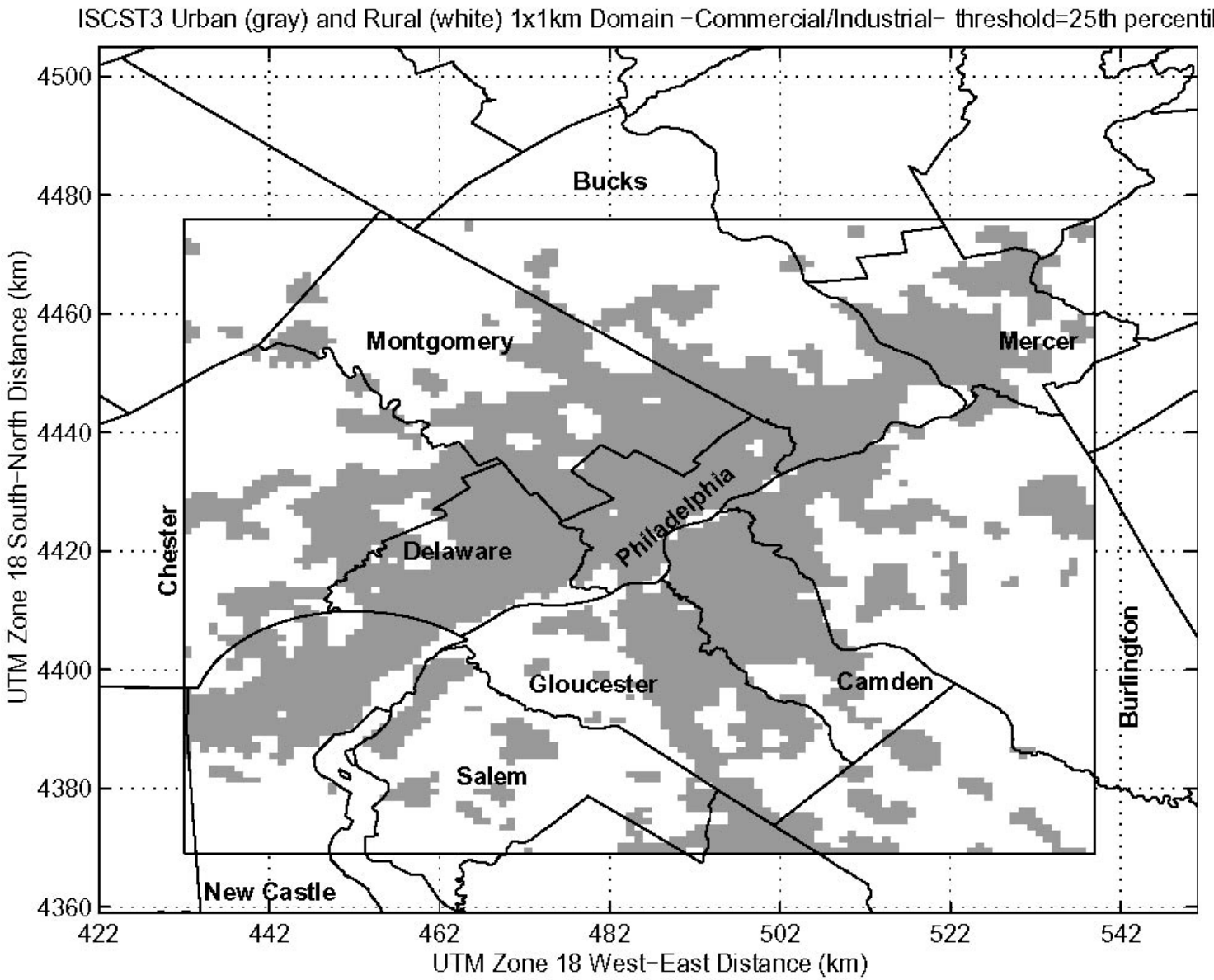
Initial modeling-related Goals of the Philadelphia Study

- 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



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

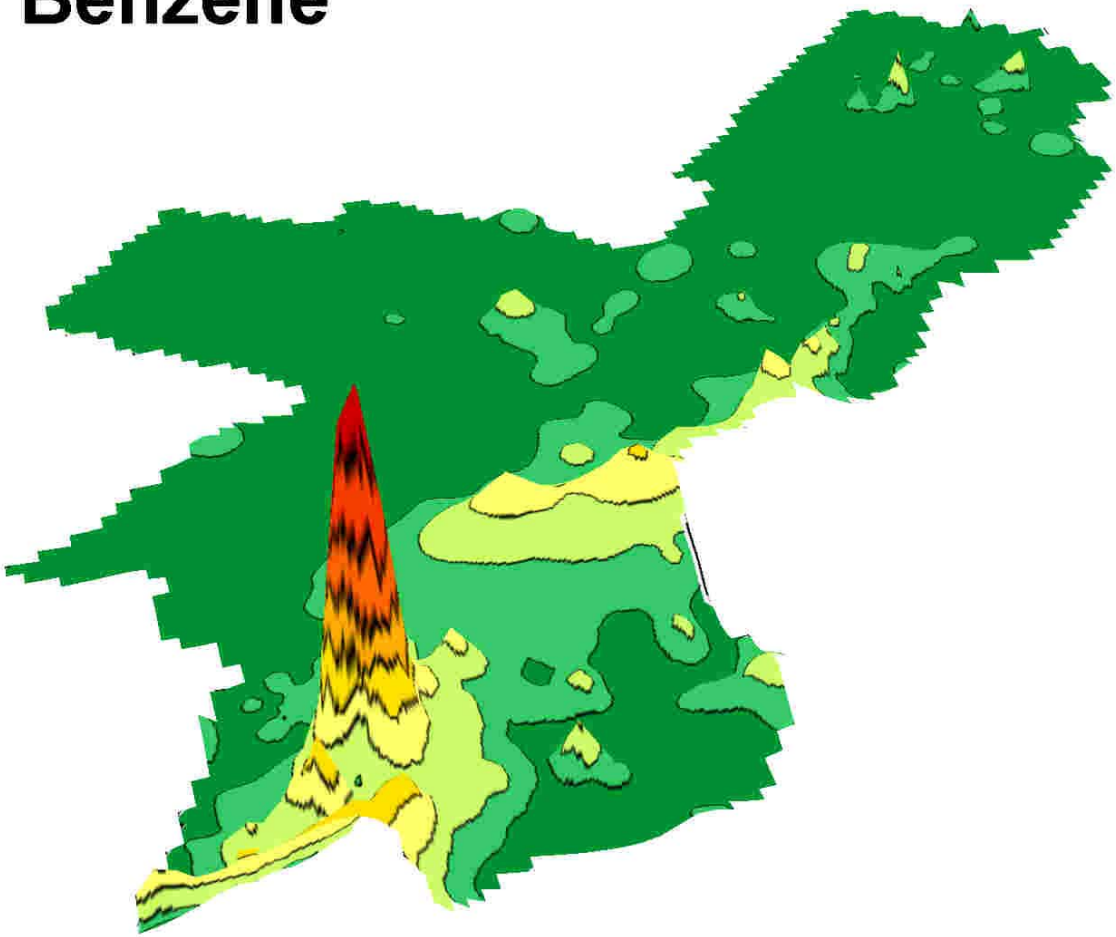
Region III

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

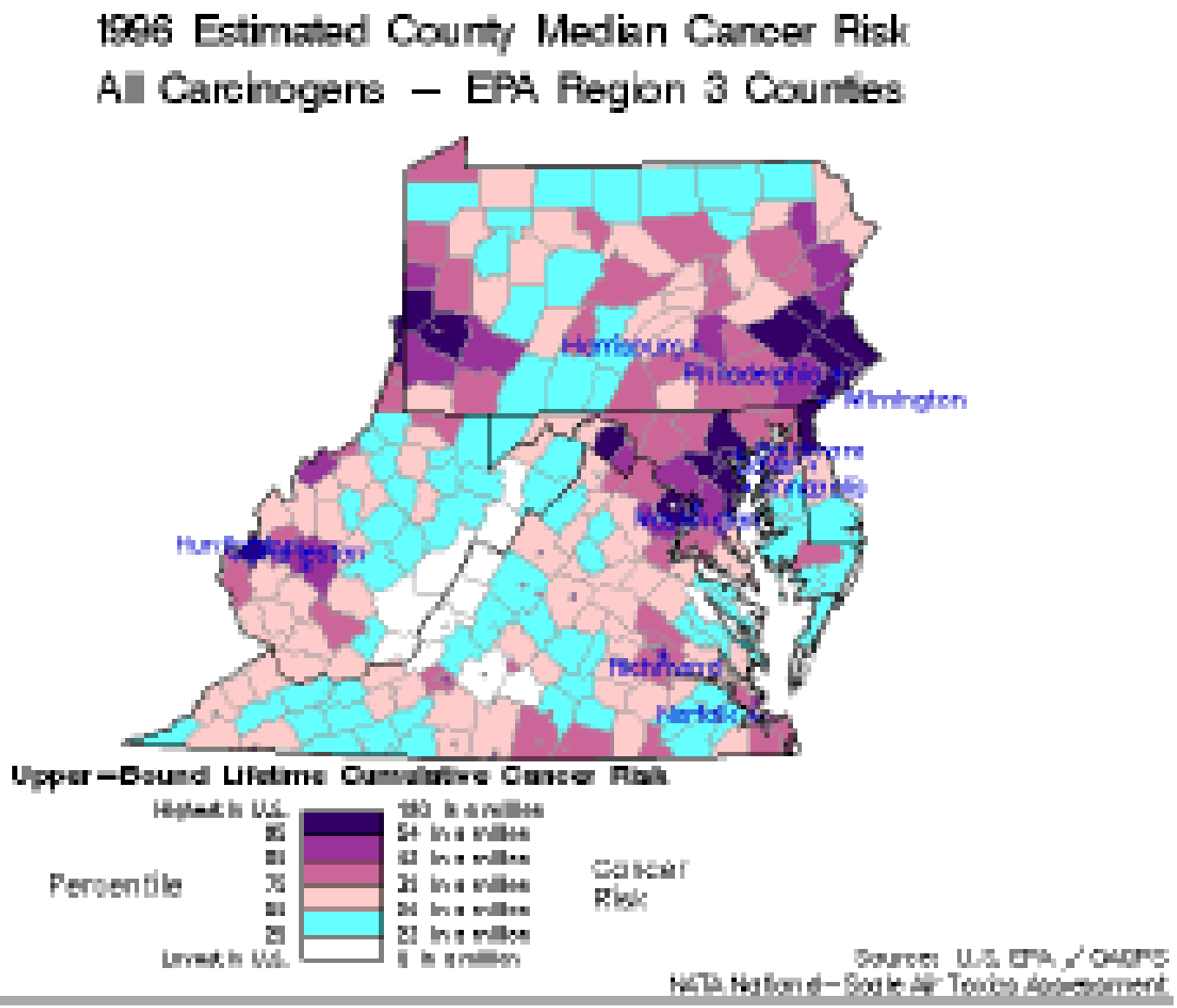
Work Completed

- 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



NATA Study Results: By County



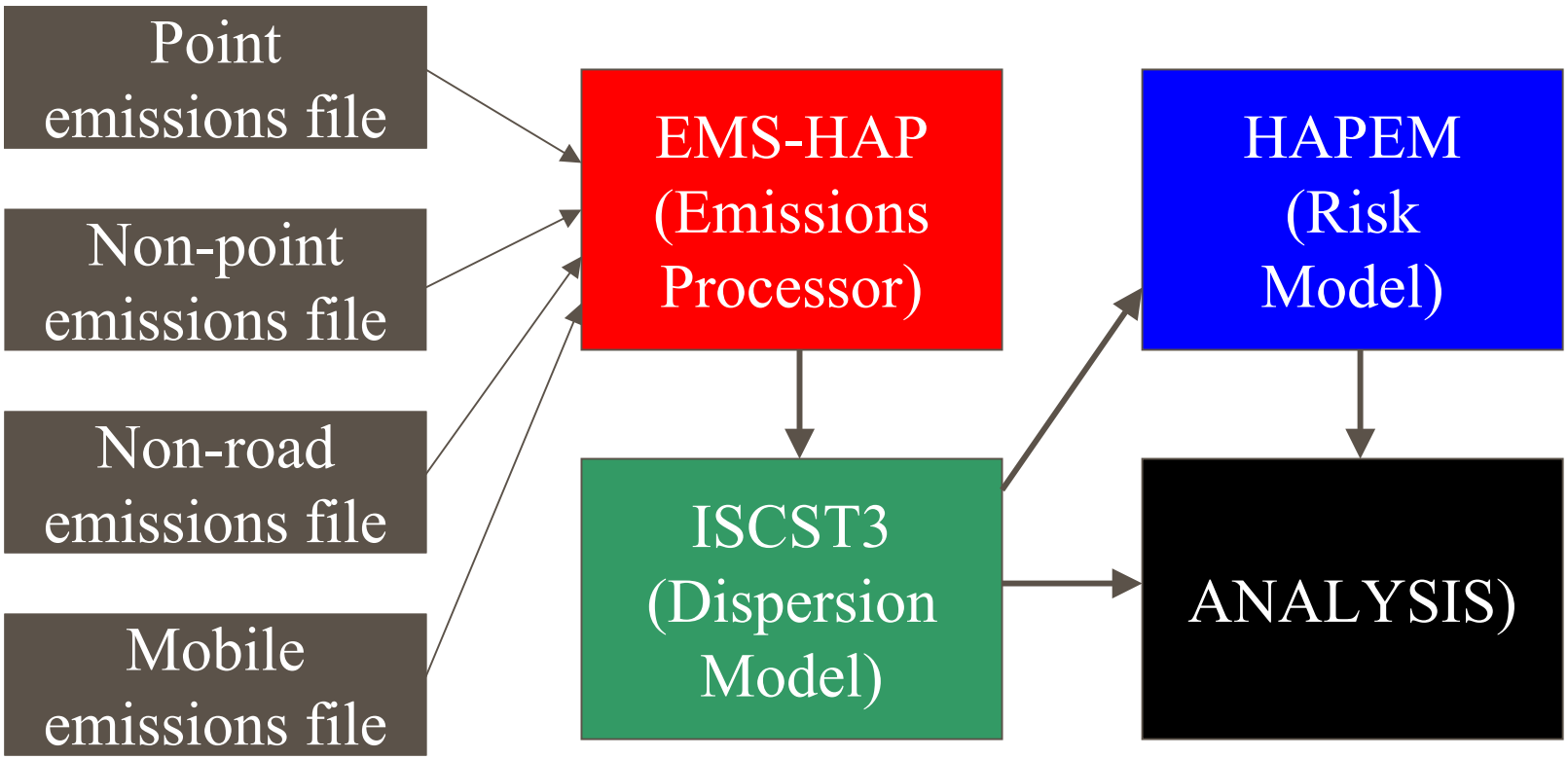
Why Modelling is More Critical for Air Toxics

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



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

Project Emissions

Assign Source Groupings

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

Functions of EMS-HAP

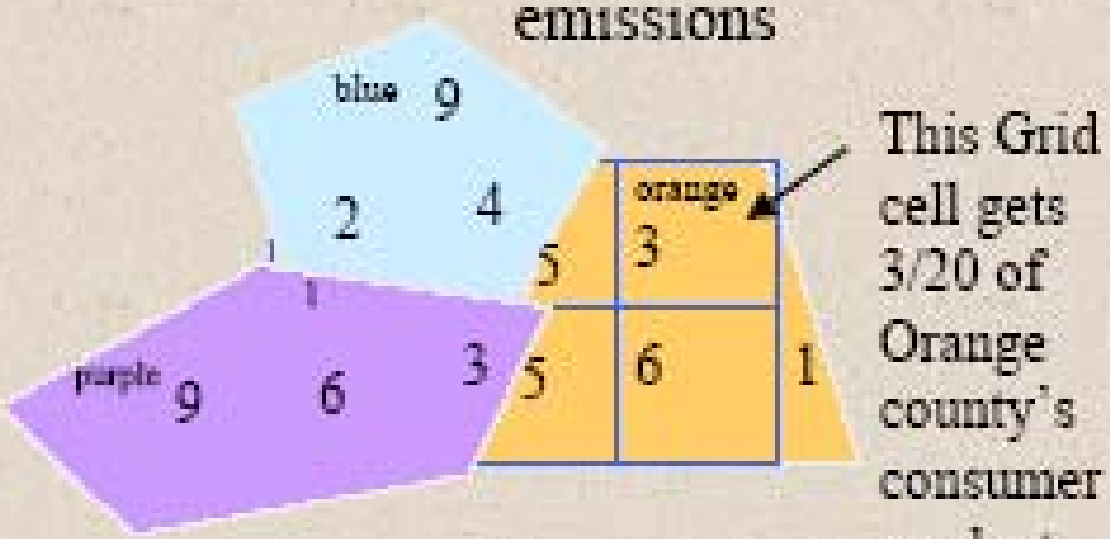
Gridded versus non-gridded Emissions

- 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



Grouping Metal Compounds for Toxics Modeling in EMS-HAP

The HAP table groups, partitions and selects pollutants

Example: Arsenic Coarse and Fine Pollutant Groups

Name of Species	Description of HAP	Inventory Pollutant Code	Reactivity	KEEP	HAP CODE	Factor
Arsenic pentoxide	Arsenic cmpds coarse	1303282	3	y	48	.2673
Arsenic acid	Arsenic cmpds coarse	1327522	3	y	48	.2164
Arsenic Trioxide	Arsenic cmpds coarse	1327533	3	y	48	.3105
Arsenic	Arsenic cmpds coarse	7440382	3	y	48	.41
Arsine	Arsenic cmpds coarse	77884421	3	y	48	.41
Arsenic & compounds	Arsenic cmpds coarse	601	3	y	48	.41
Arsenic pentoxide	**Arsenic cmpds fine**	**1303282**	**2**	**y**	**48**	**.3846**
Arsenic acid	Arsenic cmpds fine	1327522	2	y	48	.3114
Arsenic Trioxide	Arsenic cmpds fine	1327533	2	y	48	.4469
Arsenic	Arsenic cmpds fine	7440382	2	y	48	.59
Arsine	Arsenic cmpds fine	77884421	2	y	48	.59
Arsenic & compounds	Arsenic cmpds fine	1303282	2	y	48	.59

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

Speciated HAP	CAS	OldS1	NewS1	OldS2	OldS3	NewS3	SPECFX	MACT	SCC	SIC
Trivalent chromium	136	80141	5992	80341		5993	.66			
Hexavalent chromium	136	80141	6992	80341		6993	.34			
Trivalent chromium	136	80141	5992	80341		5993	.72			2431
Hexavalent chromium	136	80141	6992	80341		6993	.28			2431
Trivalent chromium	**136**	**80141**	**5992**	**80341**		**5993**	**.44**	**0107**		
Hexavalent chromium	**136**	**80141**	**6992**	**80341**		**6993**	**.56**	**0107**		

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