National Scale Air Toxics Assessment

Air Quality Modeling and Analysis Component for the Initial National Scale Assessment

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Science Advisory Board Review

March 20, 2001

Charge Question No. 2

Is the approach taken for the geographic aggregation of ambient and exposure concentrations generated by the **ASPEN** and **HAPEM4** models appropriate in light of the limitations of the models, the available emissions data, and the results of the comparisons of ambient predictions with ambient monitoring data?

Assessment System for Population Exposure Nationwide (ASPEN)

- Modeling approach reviewed by **S**cience **A**dvisory **B**oard (**SAB**) in 1996:
  - Sound overall framework
  - Importance of comparing model predictions with measured concentrations
  - Limitations in complex terrain
  - Limitations during calm conditions

Assessment System for Population Exposure Nationwide (ASPEN) (Cont'd)

- **ASPEN** model has a long history of use
- Core dispersion model based on Gaussian plume formulation: **I**ndustrial **S**ource **C**omplex **L**ong **T**erm (**ISCLT2**) model
- Nationwide assessment (using **ISCLT2**) first made in **H**uman **E**xposure **M**odel (**HEM**)
- Improvements for **S**outh **C**oast **R**isk and **E**xposure **A**ssessment **M**odel (**SCREAM2**)
- Further enhancements in **C**umulative **E**xposure **P**roject (**CEP**)

The ASPEN Model

- Suitable for national scale applications
  - Large number of sources
  - All 33 air toxics simulated together in one run
  - Concentrations calculated at census tract level
  - Concentrations calculated up to 50km
  - Computationally efficient
- Meteorological data stratified into 3-hour time blocks
- Pollutant decay, wet and dry deposition for particulates, and secondary transformation included
- Contribution from specific source categories (major, area, onroad and nonroad mobile) provided
- Background values added to **ASPEN** predicted concentrations

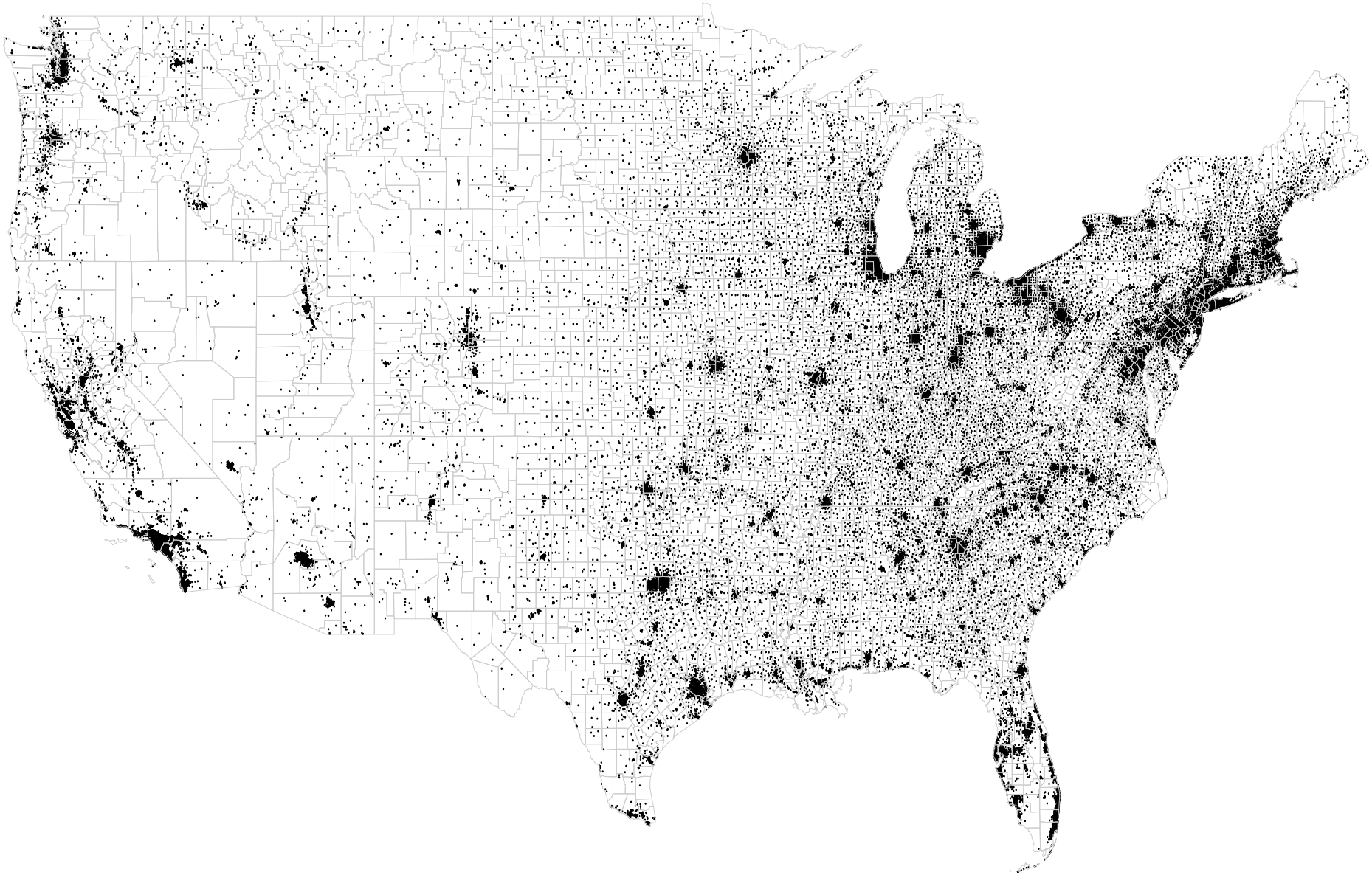
ASPEN Model Application

- Generally applied in same manner as the **CEP** study
- Few enhancements:
  - Used 1996 Emissions Inventory
  - Used all available National Weather Service meteorological stations; more representative data improve model estimates
  - Extended modeling domain
  - Estimated background concentrations for diesel PM using a modeling- based approach
  - Quality Assurance checks (scatter plots and maps); extensive reviews by State agencies

Treatment of Background

- Accounts for concentrations due to:
  - Natural sources
  - Sources not in the inventory
  - Sources located greater than 50km (long range transport)
- Values used same as previous study (technical literature)
  - Non-zero values for 13 pollutants
  - Zero for others
  - Applied uniformly across all census tracts
- Developed a modeling-based approach for diesel PM

NATA - Census Tract Centroids



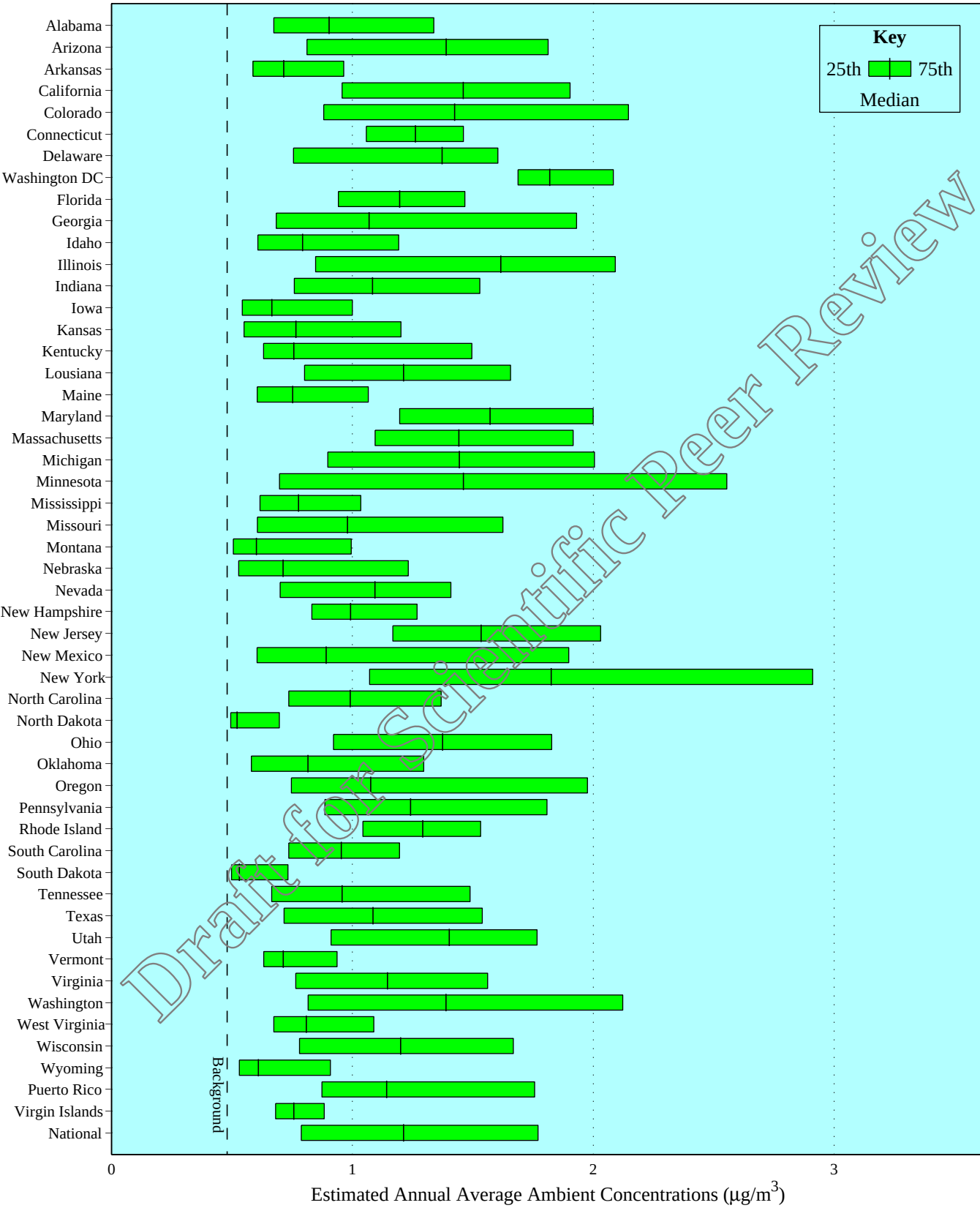
Examples of ASPEN Output

- Tables showing concentrations aggregated to county level
- Graphical output showing aggregation at State and national levels
- Contribution from specific source categories (major, area, on road and nonroad mobile, background)
- Different charts for each of the 33 air toxics

1996 Modeled Ambient Concentrations

Benzene − Statewide Estimates

This assessment has limitations (see page 2).

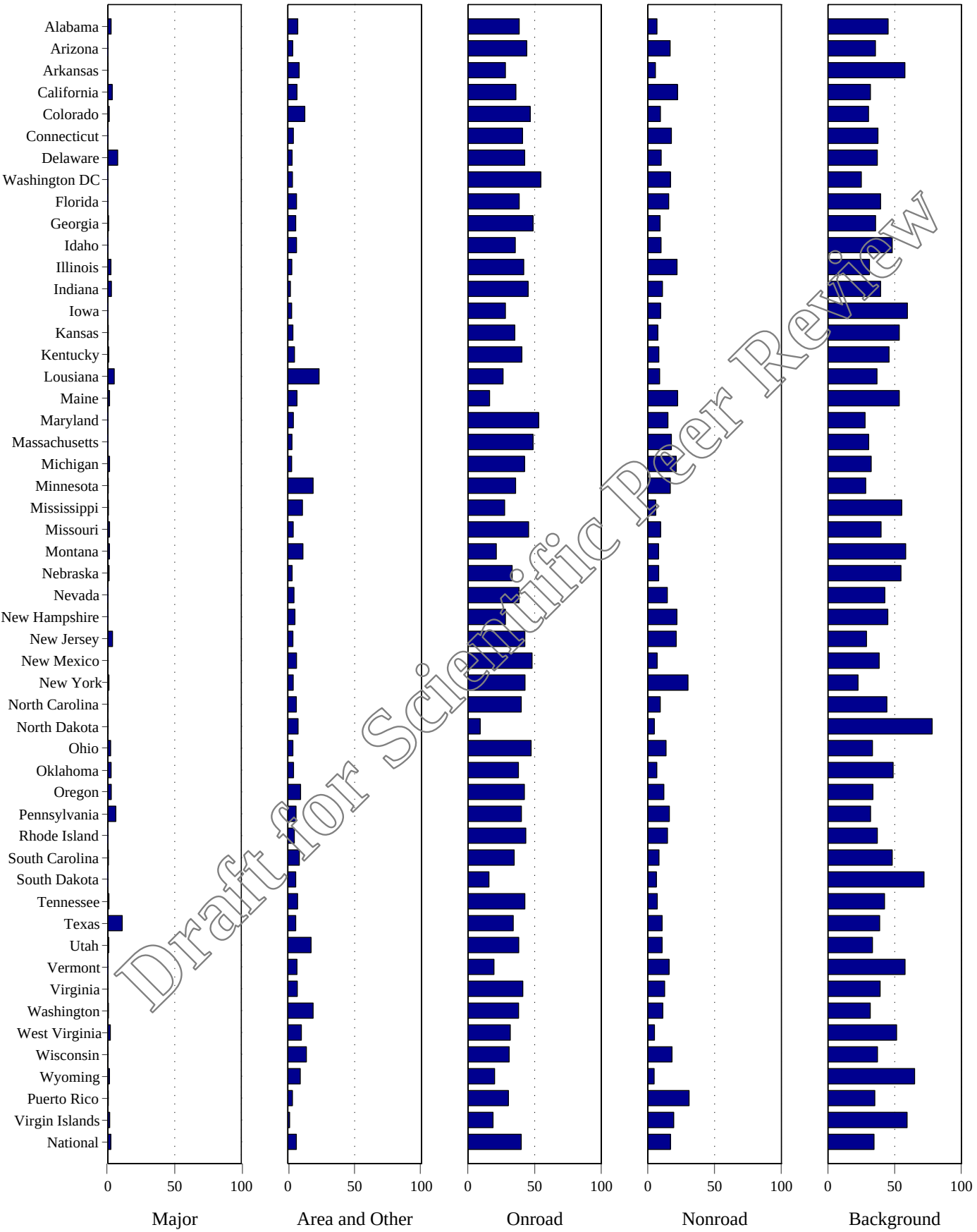


Draft for Scientific Peer Review

1996 Modeled Ambient Concentrations

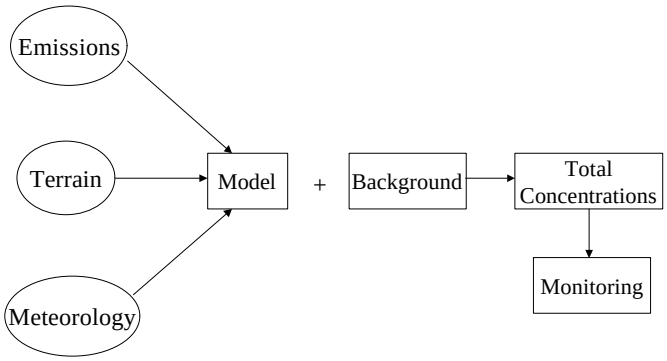
Benzene

This assessment has limitations (see page 2).

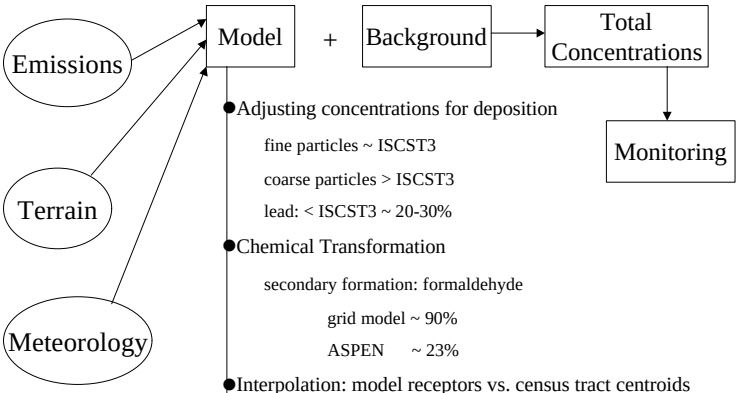


Draft for Scientific Peer Review

ASPEN Dispersion Modeling Uncertainties

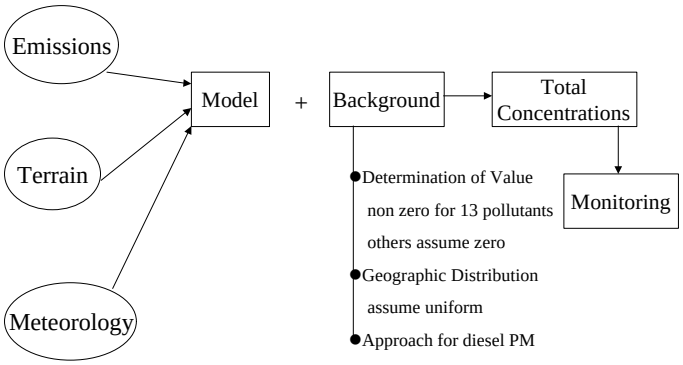


ASPEN Dispersion Modeling Uncertainties



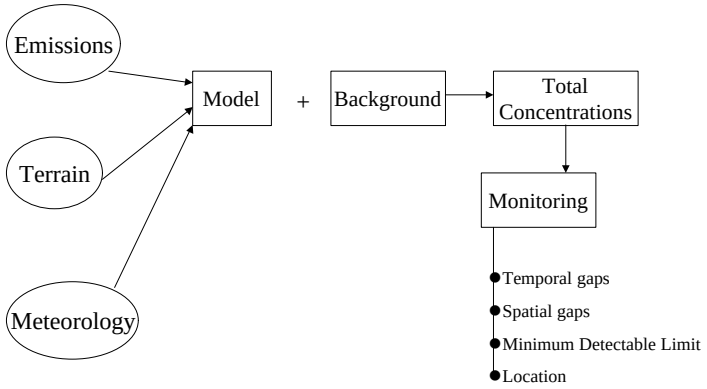
- Adjusting concentrations for deposition
  - fine particles ~ ISCST3
  - coarse particles > ISCST3
  - lead: < ISCST3 ~ 20-30%
- Chemical Transformation
  - secondary formation: formaldehyde
    - grid model ~ 90%
    - ASPEN ~ 23%
- Interpolation: model receptors vs. census tract centroids
  - ASPEN < ISCLT3 ~ 10% near field
    - < ISCLT3 ~ 25% at 30km
- Urban vs. rural tract designation

ASPEN Dispersion Modeling Uncertainties



- Determination of Value
  - non zero for 13 pollutants
  - others assume zero
- Geographic Distribution
  - assume uniform
- Approach for diesel PM

ASPEN Dispersion Modeling Uncertainties



Air Toxics Monitoring Data

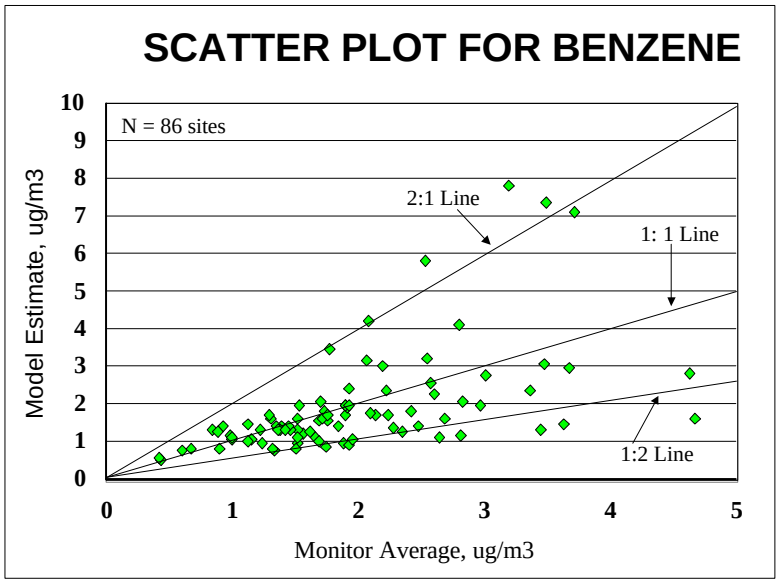
- Currently, no extensive national monitoring network
- Limited amount of monitoring data available
  - No national standards for methods, precision, and accuracy
  - Uneven geographic coverage
  - Coverage varies by pollutant
- OAQPS' Air Toxics Data Archive used for this analysis
- Data converted to annual averages to facilitate comparison to ASPEN
- Representative Air Toxics (HAPs) selected for analysis, based on available 1996 monitoring data

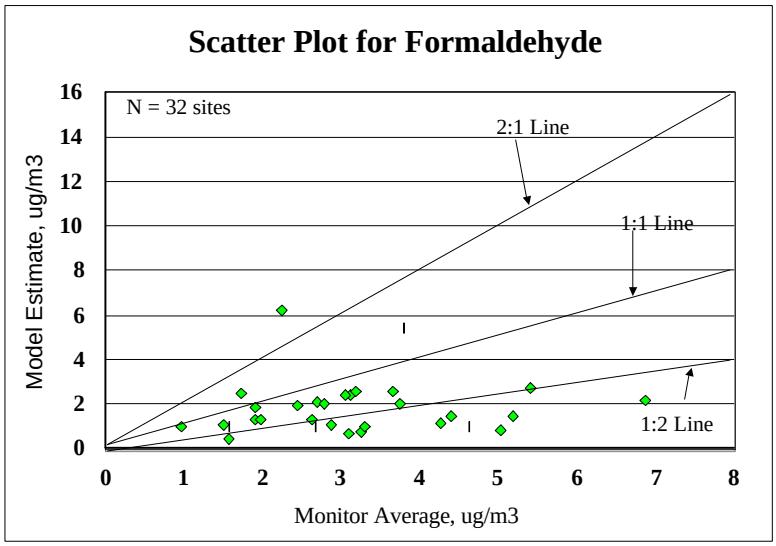
Monitoring Data Analysis Factors

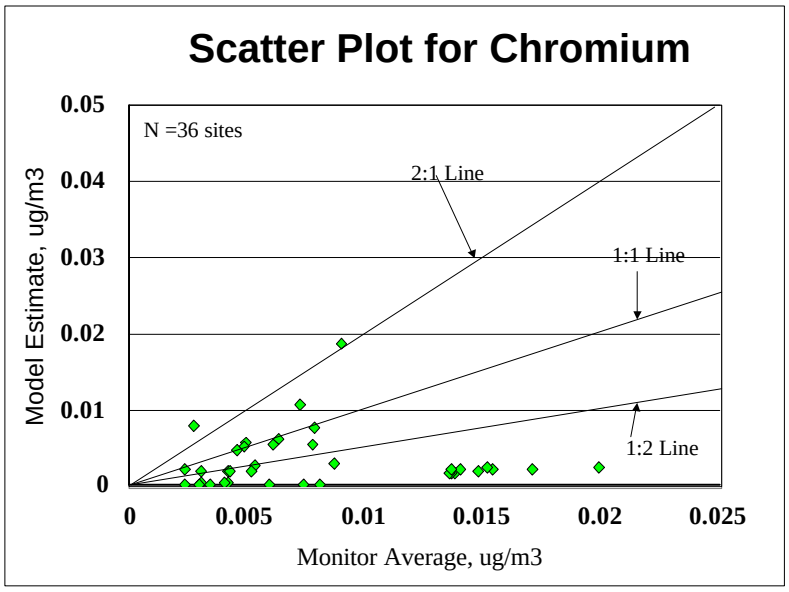
- Temporal Completeness
- Treatment of Minimum Detectable Limit (MDL) Factors:
  - Hourly and daily readings below the MDL were replaced by one-half the MDL
  - Only include pollutant/monitor combinations with at least 50% of data above the MDL
- Some monitoring data excluded

Data Analysis Techniques Used For Comparisons

- Most statistical analysis techniques reflect review by and suggestions from SAB (August, 2000)
- Most techniques deal with point-to-point comparisons
- MAXTOMON evaluates the maximum modeled concentration within a fixed distance from the monitoring location


SCATTER PLOT FOR BENZENE
N = 86 sites
2:1 Line
1: 1 Line
1:2 Line
Model Estimate, ug/m3
Monitor Average, ug/m3
0
1
2
3
4
5
6
7
8
9
10


Scatter Plot for Formaldehyde
N = 32 sites
2:1 Line
1:1 Line
1:2 Line
Model Estimate, ug/m3
Monitor Average, ug/m3
0
2
4
6
8
10
12
14
16
1
3
5
7



Point-to-Point Comparisons

Pollutant	Number of Sites	Median of Model/Monitor Ratio	Percentage of Ratios within factor of Two	Percentage of Ratios within 30%	Percentage of Ratios under-estimated by Model
Benzene	87	0.92	89	59	59
PERC	44	0.52	55	32	86
Formaldehde	32	0.65	53	28	88
Acetalaldehde	32	0.60	59	22	91
Lead	242	0.17	18	10	91
Cadmium	20	0.18	15	5	85
Chromium	36	0.15	28	19	83

MAXTOMON Statistic

Percentage of Model Estimates Underestimating Monitor Averages

Pollutant	Number of Monitors	@ 0 km (exact monitor location)	@ 10 km	@ 20 km	@ 30 km
Benzene	87	59	25	20	11
PERC	44	86	43	23	9
Formaldehyde	32	88	56	31	31
Acetaldehyde	32	91	56	38	34
Lead	242	91	65	51	40
Cadmium	20	85	60	35	25
Chromium	36	83	39	28	25

Summary and Conclusions

- Past comparisons suggest 90% of concentrations are within factor of 2
- In this analysis, model estimates of benzene compared most favorably with ambient monitored concentrations. Modeled estimates for all other HAPs typically lower than measured concentrations at exact locations of monitors.
- Comparisons improve for some of the HAPs within 10 km from the monitor site.

Summary and Conclusions (Cont'd)

- Current differences due to:
  - Model formulation
    - Deposition bias underestimates for coarse particles
    - Concentrations for reactive species are more uncertain than nonreactive
  - Meteorology
    - Reduction in average separation distance reduces uncertainty
  - Emissions
    - Uncertainties due to use of default locations
    - Unreported emissions and emission characterization
  - Background Level estimates
    - Uncertainty due to use of uniform values
- Uncertainties in monitoring data

Next Steps

- Examine model uncertainty in detail
- Refine model-based approach for estimating background concentrations
- Improve air toxics monitoring network; pilot studies underway in 4 urban and 6 non-urban areas with multiple monitor locations
- Improve emissions inventory