Development of an Anthropogenic Emissions Inventory for Annual, Nationwide Models-3/CMAQ Simulations of Ozone and Aerosols

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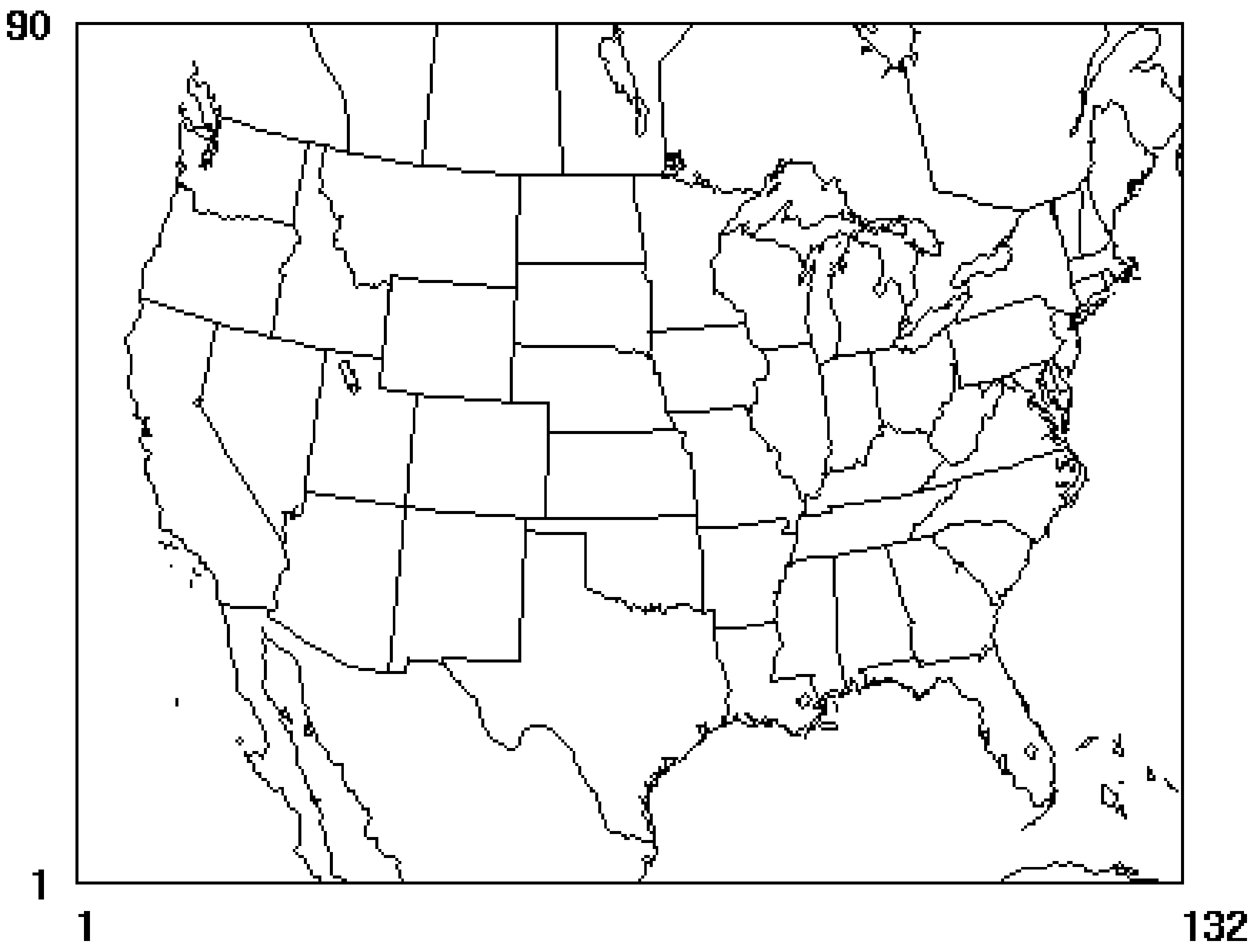
Introduction

- EPA is examining the feasibility of using the Community Multiscale Air Quality (CMAQ) Model for "one atmosphere" modeling in support of regulatory programs
  - Annual applications over a nationwide domain for 1996
  - Emissions are needed to simulate ozone, primary and secondary aerosols, acid deposition, and visibility

Overview of Presentation

- Base Emissions Inventory
- Special Considerations for Modeling Aerosols
- New Emissions-Modeling Techniques
- Enhanced Emissions QA Reports

Nationwide CMAQ Domain



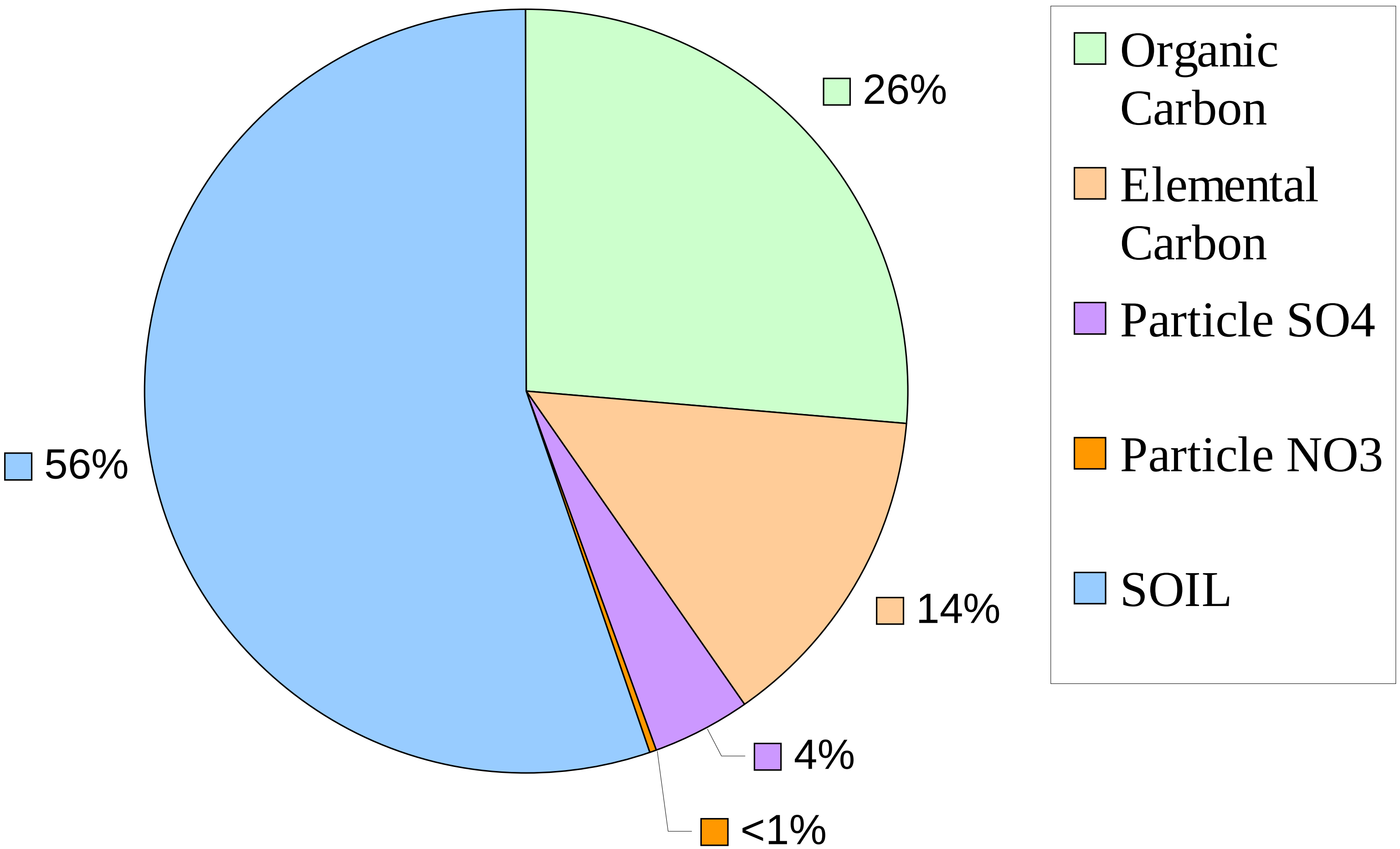
Base Emissions Inventory

- 1996 NEI v3.11 for U.S.
- Annual point/area/nonroad emissions
  - VOC, NOX, SO2, CO, PM2.5, PM10, NH3
- Monthly mobile from Heavy-Duty Engine Rule
  - Mobile5b -> “Mobile6-like” adjustments
- 1995 Canadian E/I (no point source data)

Emissions Modeling Tool

- Sparse Matrix Operator Kernel Emissions (SMOKE) Model used to generate:
  - Hourly, gridded (36 x 36 km) model-ready emissions
  - CB-IV VOC speciation & PM2.5 species

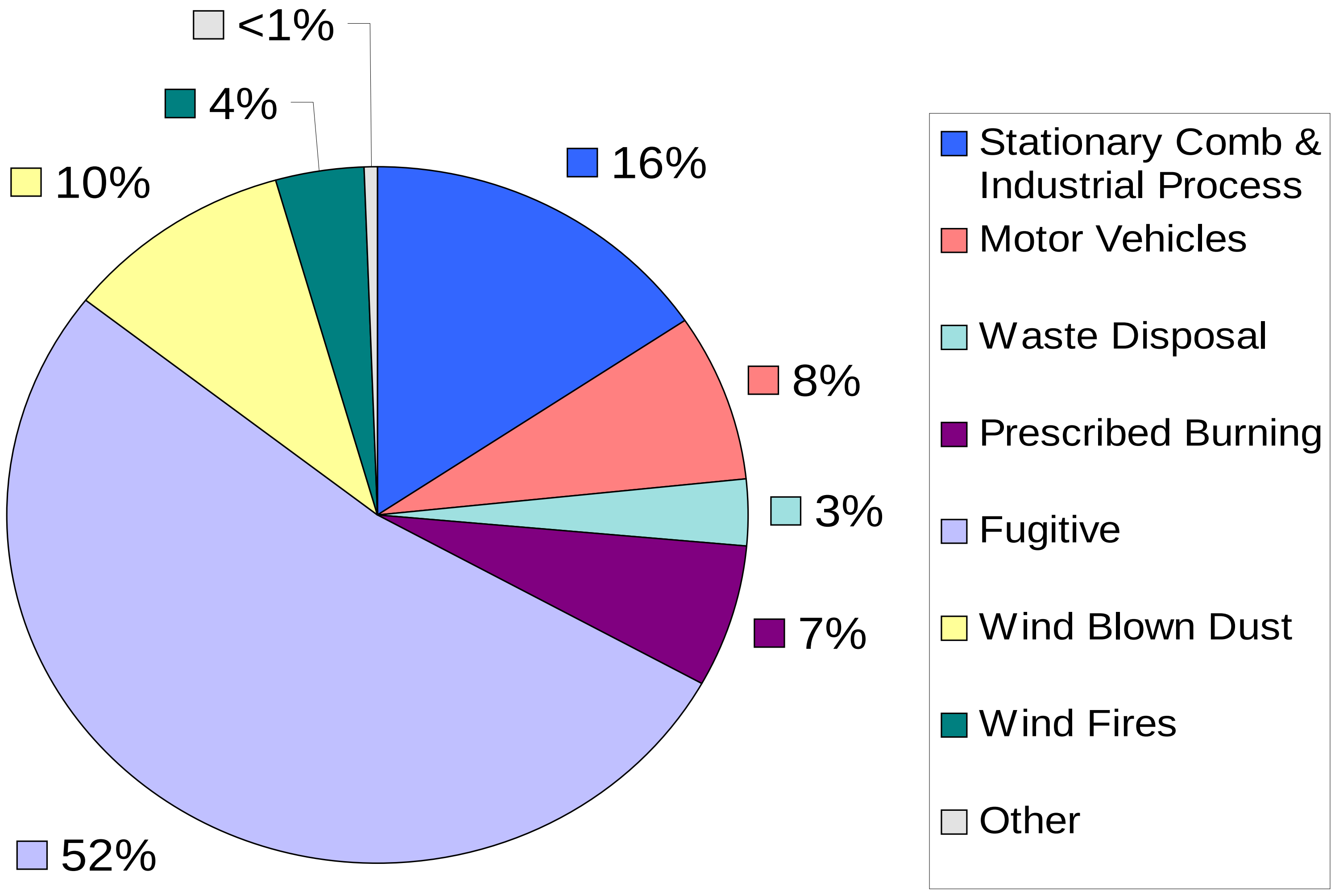
PM2.5 Emissions Species



Special Considerations for CMAQ Modeling

- Fugitive Particulate Emissions
- Wild Fires
- Wind Blown Dust
- Animal Husbandry and Fertilizer NH3 Emissions

PM2.5 Emissions
-Percent by Major Sector -



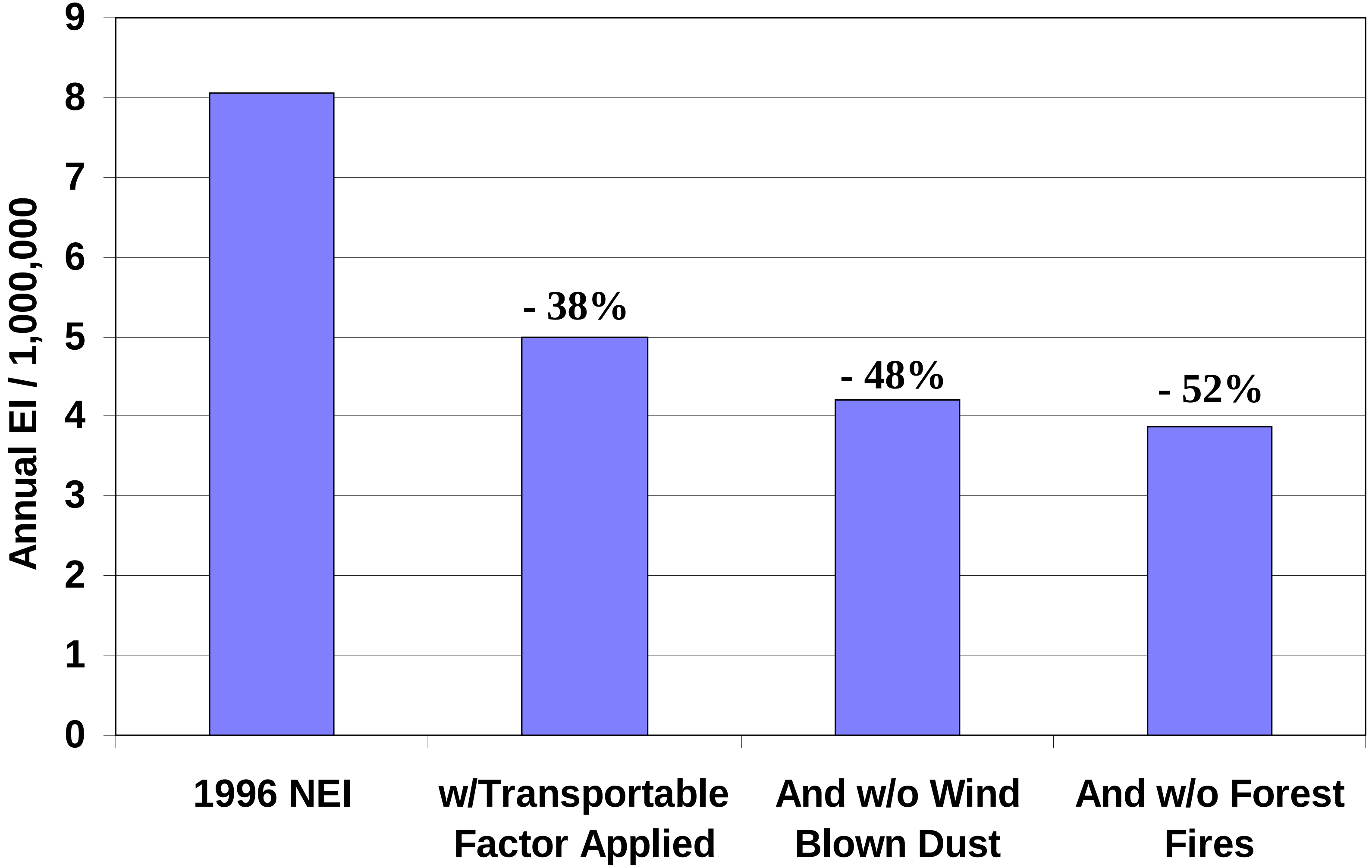
Special Considerations for CMAQ Modeling (continued)

- Fugitive Particulate Emissions
  - "Non-transportable" component of PM
    - portion of fugitive PM that settles out or impacts vegetation in vicinity of source
  - Fugitive PMCoarse and PM2.5 reduced by 75%
    - Paved Roads
    - Unpaved Roads
    - Unpaved Airstrips
    - Agriculture Production
    - Construction

Special Considerations for CMAQ Modeling
(continued)

- Wind Blown Dust and Wild Fires
  - Difficult to take annual total emissions and determine when emissions actually occurred during the year
  - For this application, emissions from these categories were excluded from model simulations

PM2.5 Emissions (tons)

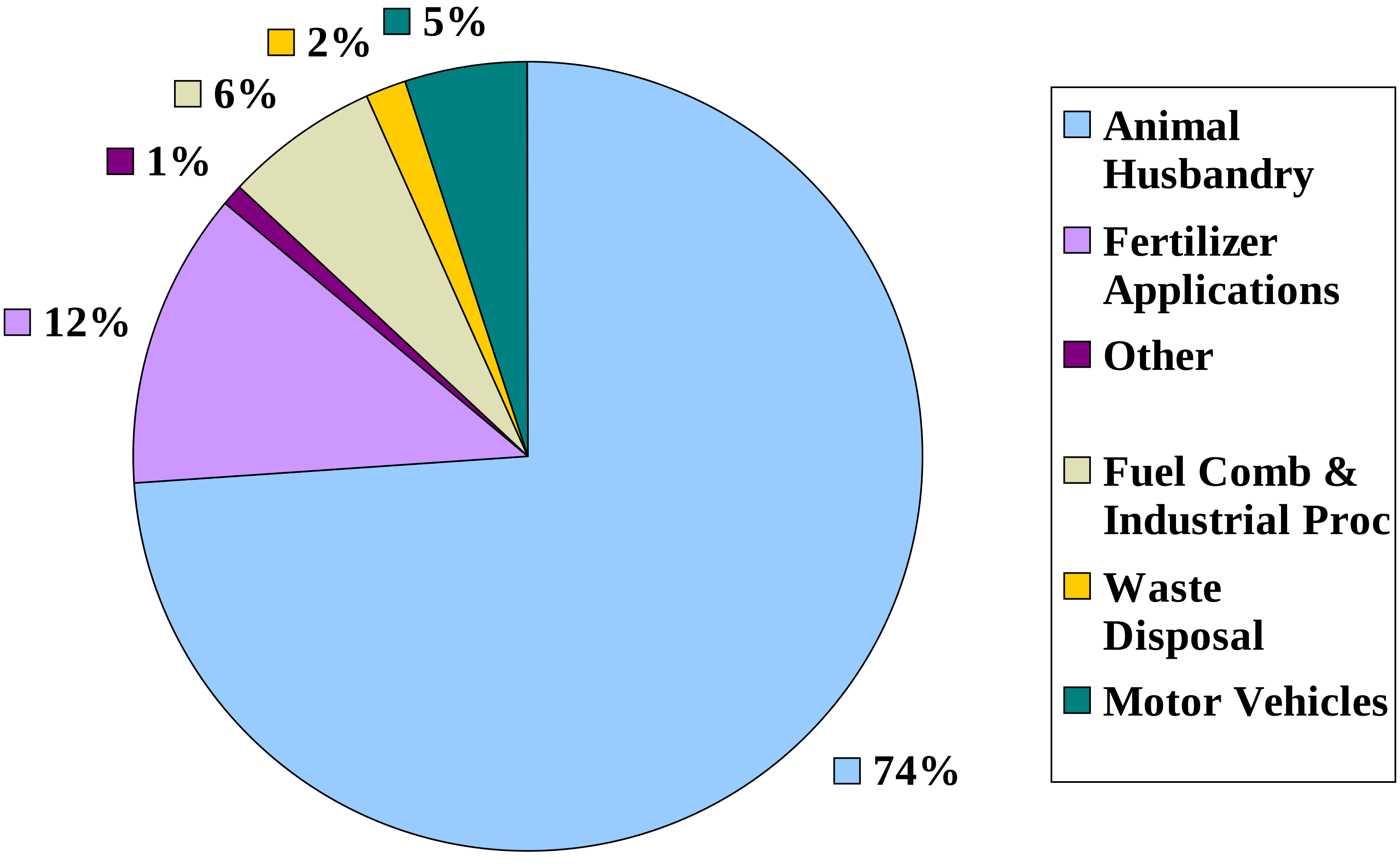


Special Considerations for CMAQ Modeling

(continued)

- Animal Husbandry and Fertilizer NH_3 E/I

NH3 Emissions - Percent by Major Sector-



Special Considerations for CMAQ Modeling

(continued)

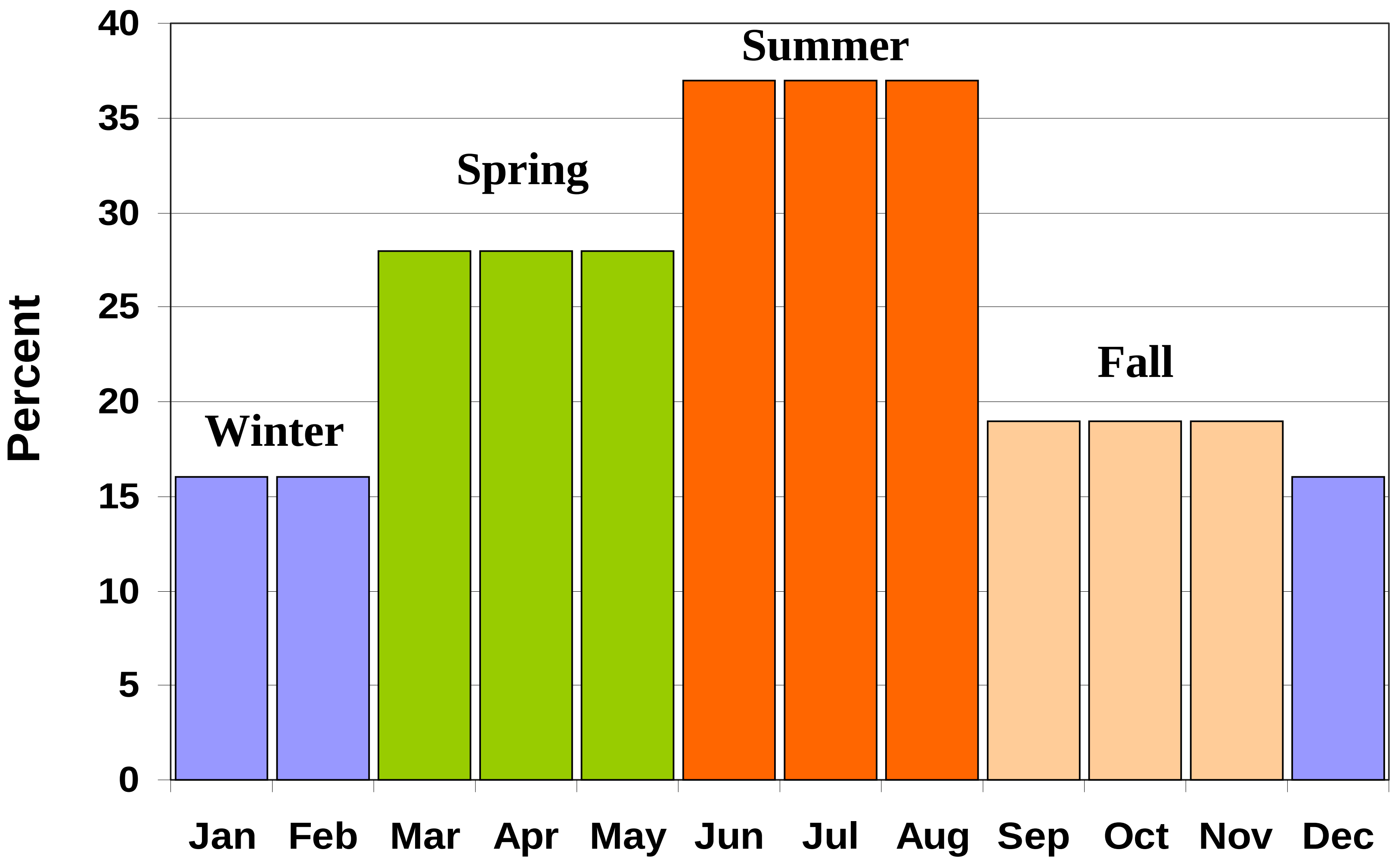
- Animal Husbandry and Fertilizer NH3 E/I
  - Annual NH3 emissions had been allocated uniformly, 25% in each season
  - Seasonal profiles were used in this study to improve characterization of NH3 emissions
    - Emissions from lagoons, housing, fields sensitive to temperature and moisture
    - Emissions from fertilizer applications also sensitive to when fertilizer is applied to soil

Seasonal Distribution of NH3

Source Category	Winter	Spring	Summer	Fall
Animal Husbandry	15%	25%	40%	20%
Fertilizer Application	10%	50%	30%	10%

Percent of NH3 By Month

(all categories combined)



New Techniques

- Gridded Surrogates for Mobile Emis/VMT
  - Prior modeling used population to grid emissions/VMT for all roadway types except interstates
  - New Method
    - Mobile emissions/VMT broken out into six roadway types (urban/rural classes for primary, secondary and local roads) using TIGER roadway links and urban/rural area designations

New Techniques
(continued)

- Estimation of Sulfuric Acid Vapor Emissions
  - Previously, SOX emissions were speciated as 97% SO2 and 3 percent gaseous sulfate (sulfuric acid)
  - However, SO2 (not SOX) is generally reported in the NEI.
  - New method was developed to estimate gaseous sulfate based on the fractions of sulfur emitted as SO2 and as gaseous sulfate

New Techniques

(continued)

- New method assumes that that gaseous sulfate emissions are primarily H_2SO_4

- $H_2SO_4 = SO_2 \times R1 \times R2$
  - R1 = ratio of sulfur emitted as sulfate to that emitted as SO_2
  - R2 = ratio of molecular wgts of H_2SO_4 to SO_2

- H_2SO_4 calculated by fuel type for certain combustion sources

Fraction of Sulfur Emitted as SO2 and Gaseous Sulfate

Fuel Type	*Fraction SO2*	*Fraction Gaseous Sulfate*	*Remaining (ash)*
Bituminous Coal	0.950	0.014	0.036
Sub-Bituminous Coal	0.875	0.014	0.111
Lignite Coal	0.750	0.014	0.236
Residual Oil	0.990	0.010	0.000
Distillate Oil	0.990	0.010	0.000

Enhanced SMOKE QA Reports

- User-defined reports can be generated before/after the major steps in emissions processing (i.e. import, temporal, spatial, speciation, and merge)
- Reports available in printable format or for import into spreadsheets

Enhanced SMOKE QA Reports

(continued)

- Reports can be created by:
  - country, state, county, grid cell
  - geographic groupings
  - annual, daily, hourly
  - major category (area, mobile, point)
  - road class or 10-digit SCC
  - individual source for point sources (plant name and stack parameters)
  - elevated or only Plume-in-Grid point sources
  - pollutant species (mass or moles)
  - spatial surrogate for area and mobile sources

Conclusions

- For regional/national aerosol modeling….
  - Need to consider potential inconsistencies between annual mass inventories and the nature of the model application
    - Using mass emissions for fugitive categories could greatly overestimate what is transported beyond the immediate area of the source
    - Using an annual inventory makes it difficult to capture the actual occurrence of emissions for episodic or periodic source types like wind blown dust and wild fires

Conclusions

(continued)

- Additional improvements needed for temporally allocating NH3 emissions
- New techniques for gridding mobile source emissions and for estimating emissions of H2SO4 may help to improve modeling results