EPA's Multipollutant Modeling with the 2002 NEI: Integrating Criteria and Toxics

Emission Inventory Conference

New Orleans, May 18, 2006

Madeleine Strum, USEPA/OAQPS

Co authors: Marc Houyoux (OAQPS), Rich Mason*
Allan Beidler and Cliff Stanley (Computer Sciences Corporation),
Deborah Luecken (USEPA/ORD)

***Atmospheric Sciences Modeling Division, Air Resources Laboratory, NOAA, (On Assignment to OAQPS)**

Why multipollutant modeling and assessment capability?

- It is the future of the Air Quality Management system
- Responsive to AQM Recommendations
  - Strengthen scientific and technical capacity
    - 1.5 Framework for Accountability
  - Develop an integrated program for criteria pollutants and hazardous air pollutants
    - 4.1 Multi-pollutant SIPS
    - 4.2 Multi-pollutant benefits and disbenefits in standard setting

"One-Atmosphere" Management and Modeling

Mobile Sources

NOx, VOC, PM, Toxics

(Cars, trucks, planes, boats, etc.)

Industrial Sources

NOx, VOC, SOx, PM, Toxics

(Power plants, refineries/ chemical plants, etc.)

Nonpoint Sources

NOx, VOC, PM, Toxics

(Residential, farming commercial, biogenic, etc.)

Chemistry

Meteorology

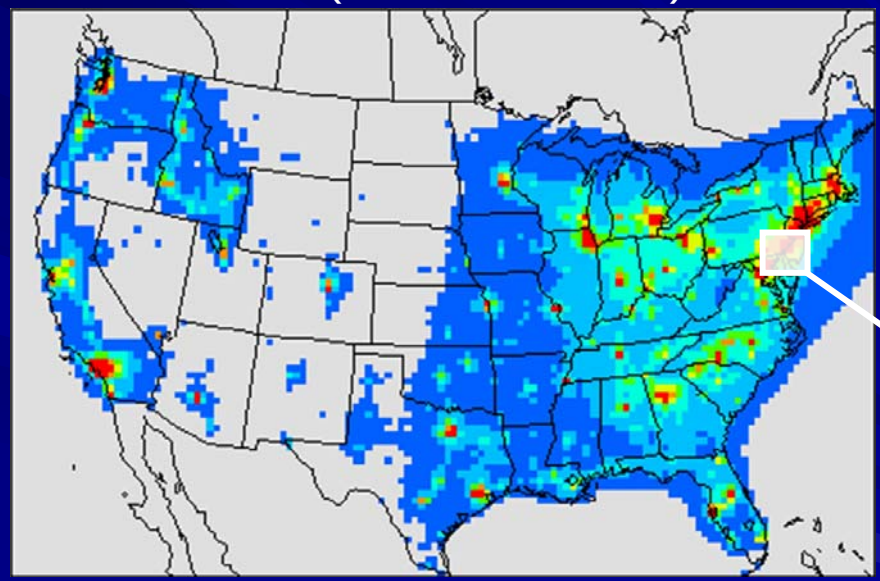
- Ozone
- PM
- Acid Rain
- Visibility
- Air Toxics
- Atmospheric Deposition
- Climate Change

Multipollutant Modeling Capability For Strategy Analysis: Illustrative Example

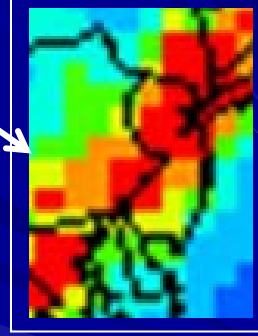
Possible Strategy:
Pulp and Paper
Flue gas desulfurization (wet scrubber) limit SO2 to 2 lb/ ODTP (oven-dried tons pulp production)
Resulting reductions (industry average)

Pollutant	Reduction
SO2	78%
PM25	99%
Organic HAP	89 to 94%
non-hg metal HAP	70 to 99%
HCl	100%
Hg	70-90%

Nationwide CMAQ Predicted Change in Pollutant (ozone/PM/toxic)



Philadelphia county



What has been done?

- Added toxics to CMAQ
  - 20 VOC HAPs added through development of CB4tx, SAPRCtx mechanisms
- Updated SMOKE to process HAPs and combine HAP/CAP inventories
- Modeled HAPs in CMAQ (1999 NEI)
- Made NEI more consistent across CAPs and HAPs

What are we doing now?

- Adding even more toxics to CMAQ
  - Nearly 40 HAPs being added through CB05tx mechanism
- Preparing 2002 NEI and ancillary files needed to implement HAP/CAP combination approach

A Look at Selected* (Organic Gas-phase) CB05 Model Species

CB05 Model species	Description	Active HAP?
FORM	formaldehyde (explicit)	yes
ALD2	acetaldehyde (explicit)	yes
ALDX	lumped C3+ aldehydes	
CH4	methane (explicit)	
ETHA	Ethane (explicit)	
PAR	1-carbon paraffin	
ETH	Ethene (explict)	
OLE	terminal olefins	
IOLE	internal olefins	
TOL	toluene (7 carbons) KOH=8.8E3	
XYL	xylenes (8-carbons) KOH=3.7E4	
ISOP	Isoprene (explicit)	
MEOH	Methanol (explicit)	yes
ETOH	Ethanol (explicit)	
TERP	lumped terpene species	

* See paper for full list

A Look at Selected* CB05tx "Tracer" HAPs

Organic and other gases

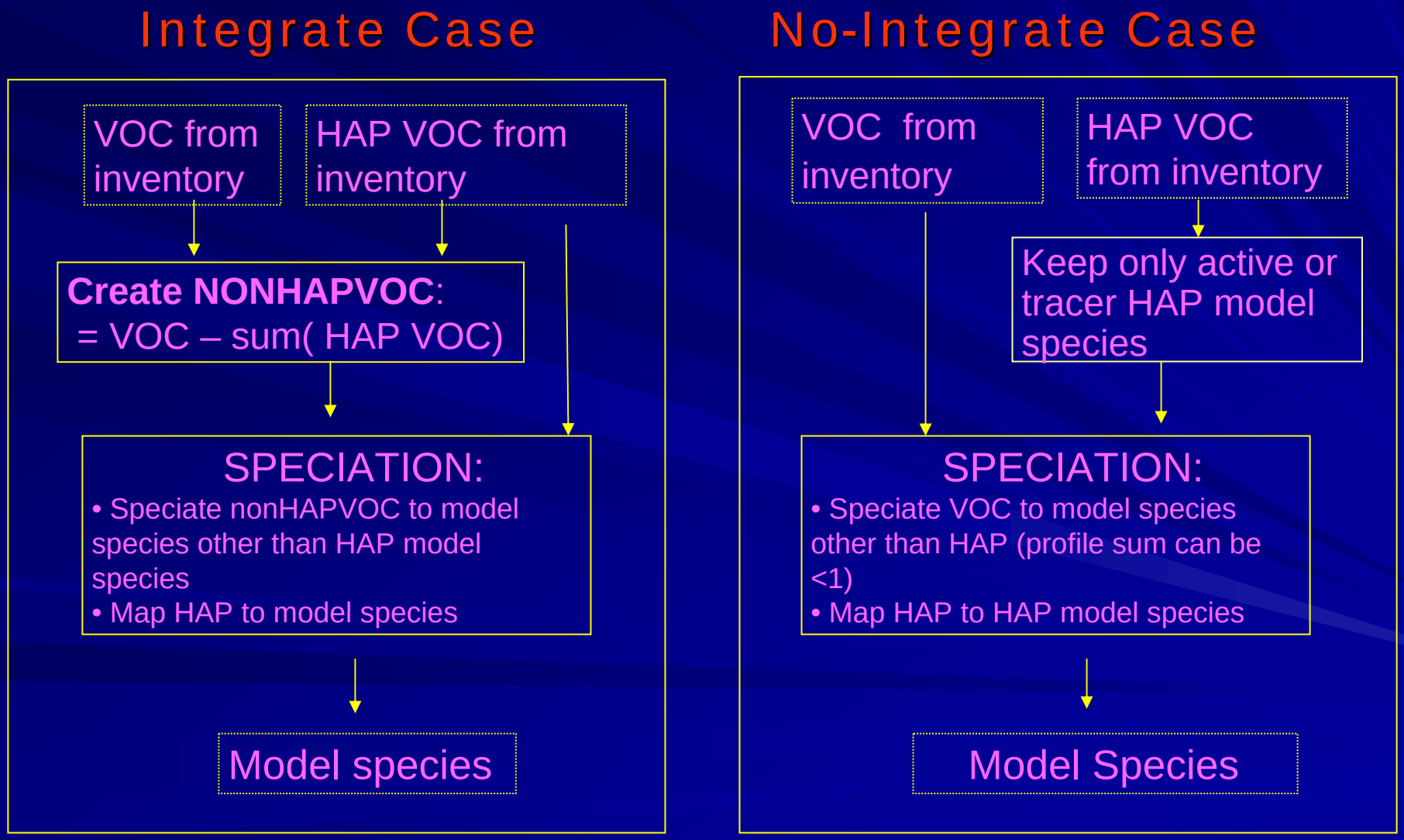
CB05tx Tracer Toxics	Name
Cl2	molecular chlorine
HCL	hydrochloric acid
BUTADIENE13	1,3-butadiene
ACROLEIN	acrolein
NAPTHALENE	naphthalene
BENZENE	benzene
PROPDICHLORIDE	1,2-dichloropropane
CL4_ETHE	Tetrachloroethylene (perc)
CARBONTET	carbon tetrachloride
CL2_ME	methylene chloride
CHCL3	chloroform
TRIETHYLAMINE	Triethylamine

* See paper for full list

Diesel PM & metals

CB05tx Tracer Toxics	Name
diesel_pec	**Diesel PM - elemental carbon**
diesel_poa	**Diesel PM - organic carbon**
diesel_pso4	**Diesel PM - sulfates**
diesel_pno3	**Diesel PM - nitrate**
diesel_pmfine	**Diesel PM - other fine particulate**
diesel_pmc	**Diesel PM - coarse particulate**
beryllium_coarse	**Beryllium compounds - fine particulate**
beryllium_fine	**Beryllium compounds - coarse particulate**
cadmium_coarse	**Cadmium compounds - coarse particulate**
cadmium_fine	**Cadmium compounds - fine particulate**
PLUS: Lead, manganese, nickel, hexavalent chromium, trivalent chromium	

Two Ways to Combine HAP/CAP Using the HAP inventory



Determining Sources in 2002 NEI that could use the Integrate case

- 1) All VOC HAPs and VOC are uniformly submitted by the State or are computed by EPA;
- 2) The sum of VOC HAPs is less than or equal to the VOC.
- 3) The particular VOC HAPs can be mapped to model species.

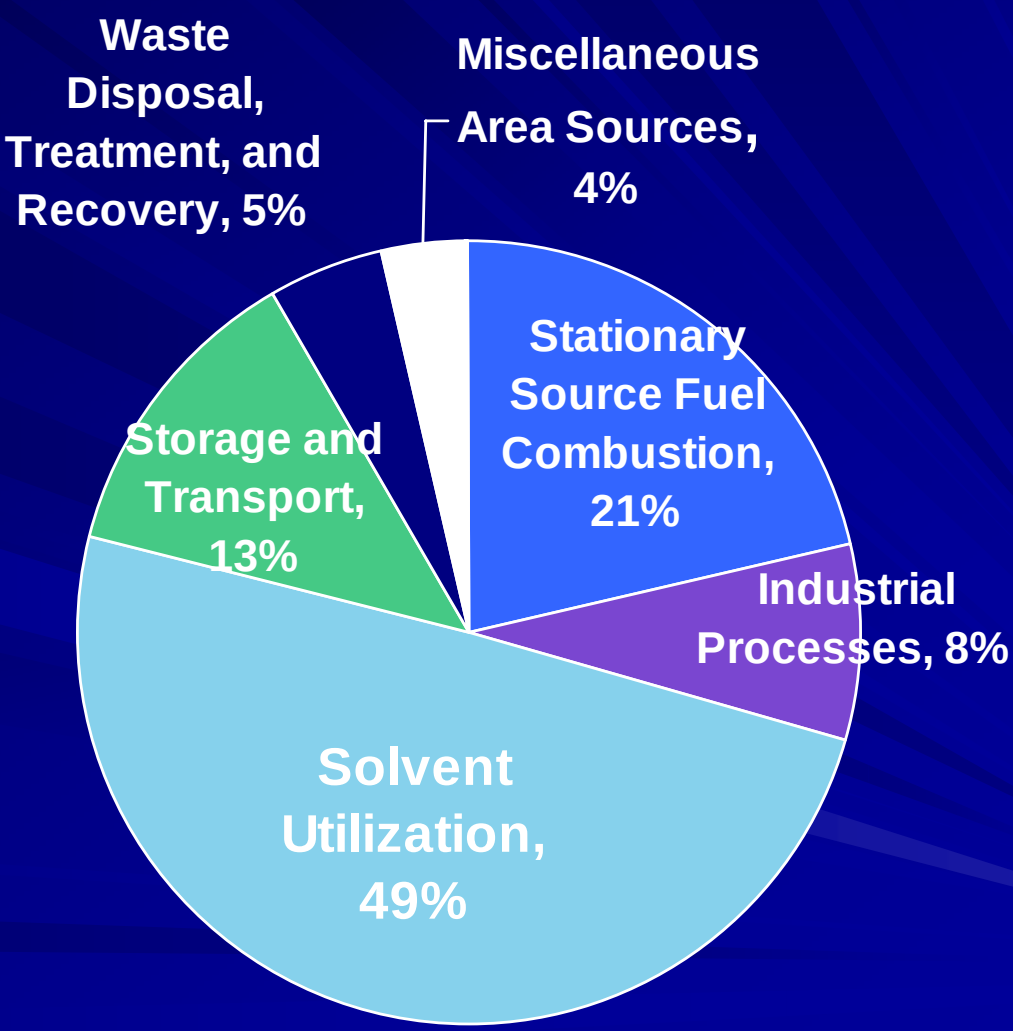
Inventory Analysis Covered Largest VOC sources

- Analyzed:
  - Nonpoint (8 million)
  - Onroad (4.6 million)
  - Nonroad* (3 million)
- Did yet not analyze
  - Point (1.7 million)
  - Point fires wild & prescribed
  - aircraft, locomotives commercial marine (.1 million)

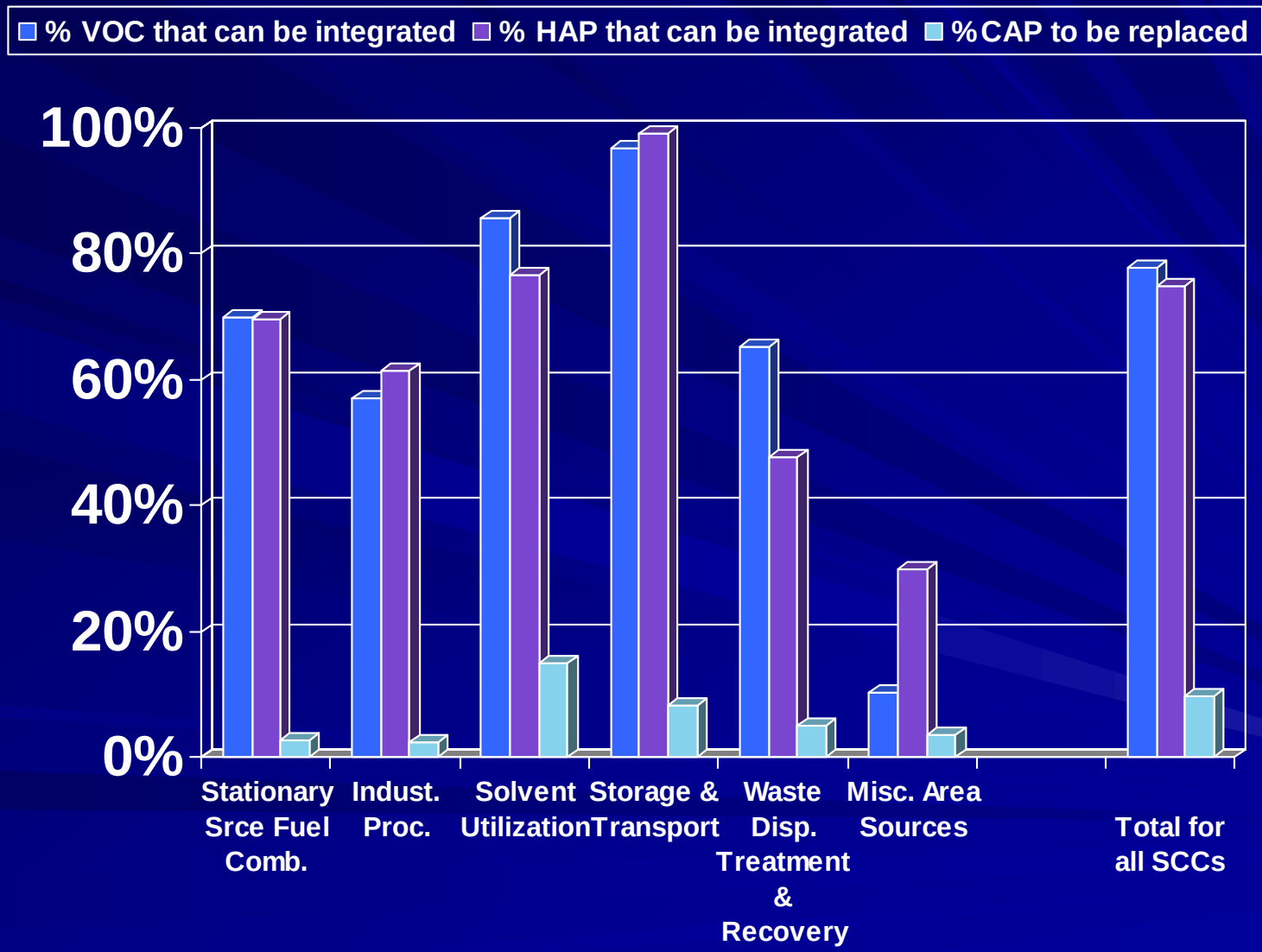
* excluding aircraft, locomotives commercial marine)

Nonpoint

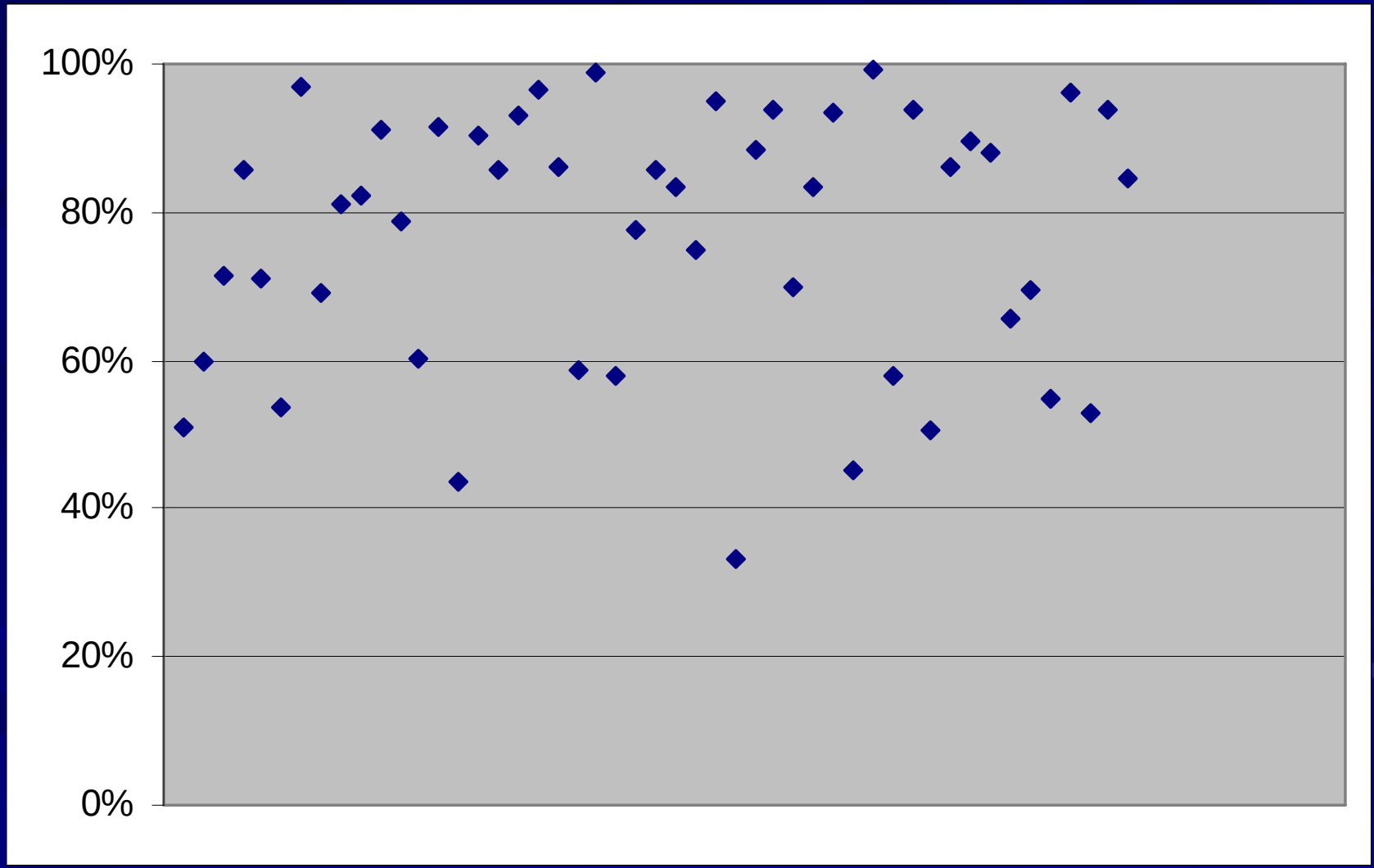
- Contains nearly 400 SCCs covering a wide range of emission processes
- Pie chart shows % of VOC by “tier 1” grouping



Nonpoint –Integration status



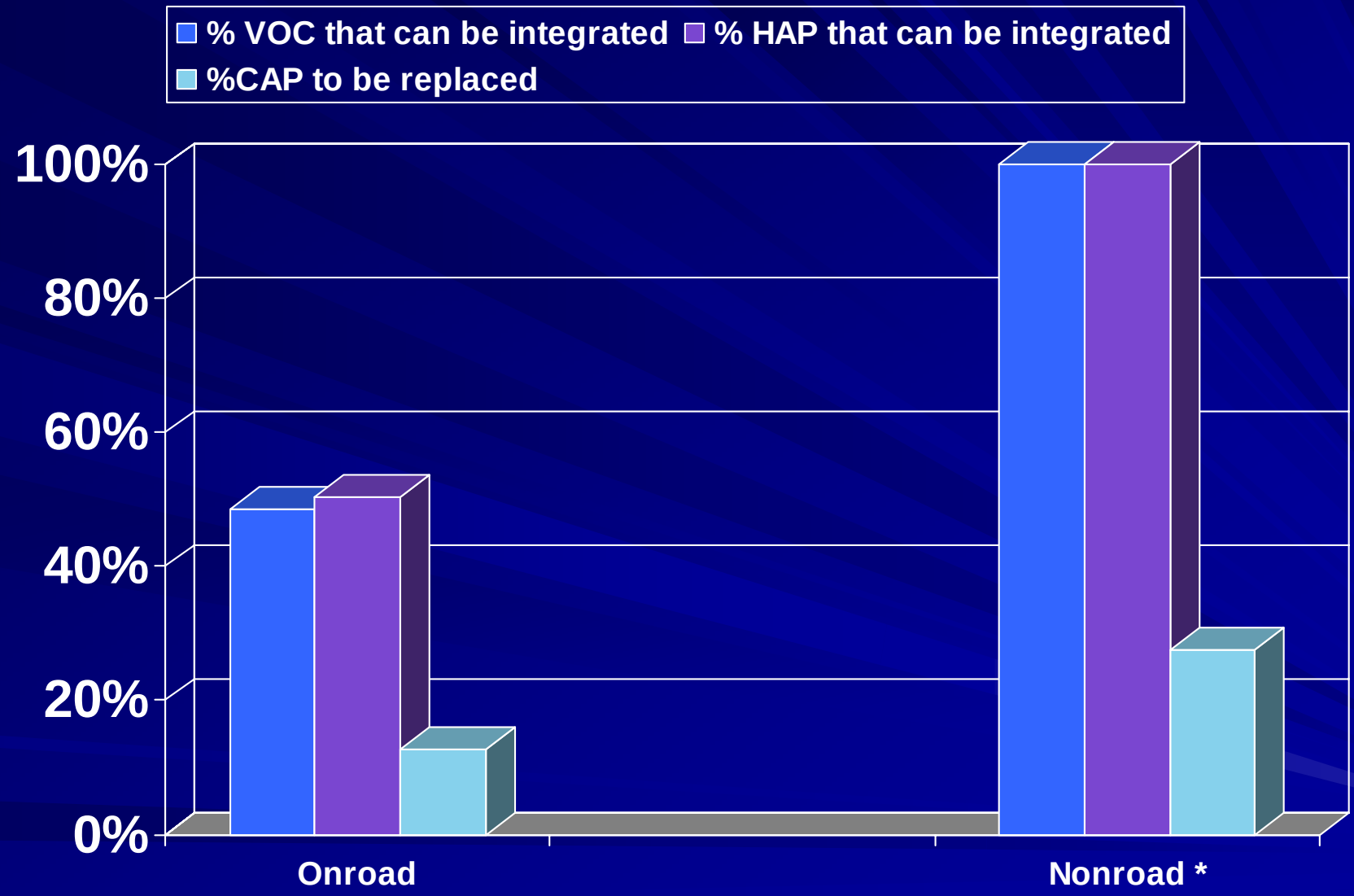
Variability in the Nonpoint %VOC in the "Integrate" Case Across States



Mobile

- Onroad: “Integrate” sources require consistent methodology across VOC and each VOC HAP
  - NMIM with EPA default inputs
  - NMIM with State supplied inputs
  - State data replacing NMIM based on EPA default inputs
  - State data replacing NMIM based on state supplied inputs
- Nonroad (excluding aircraft/CMV/locomotives): 100% “Integrate”

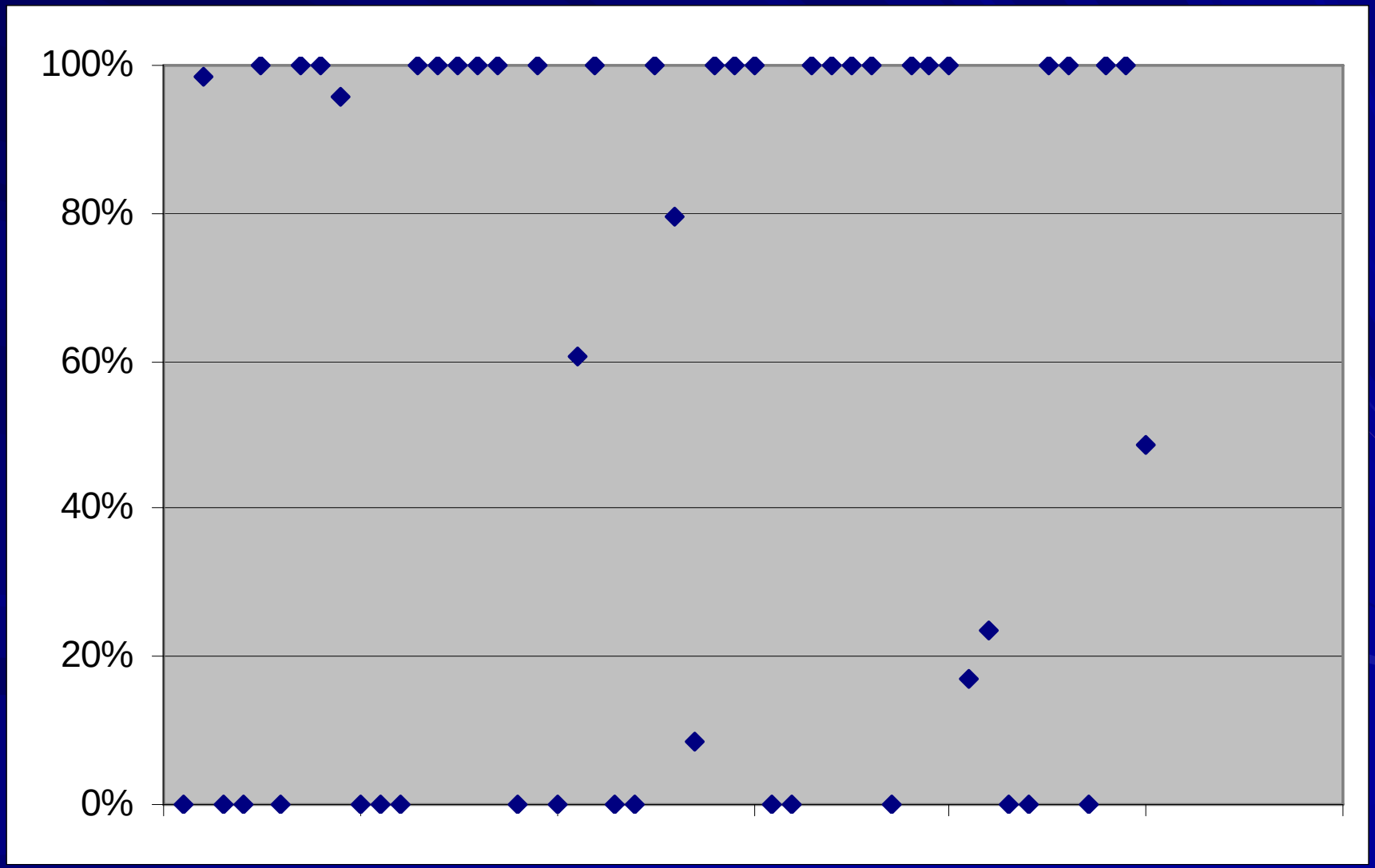
Mobile –Integration status



Note: consistent across Onroad vehicle types except diesel has slightly lower % CAP replacement (8% vs 12.8%)

* Excludes aircraft/loco/CMV

Variability in the Onroad %VOC in the “Integrate” Case Across States



Particular HAPs that Can be Integrated

Onroad/Nonroad: ~ 30 HAPs

Nonpoint: ~100 HAPs

Key HAPs: toluene, xylenes, benzene, methanol

Limitations

- We assume HAP estimates are better than speciating VOC
- We assume we can subtract HAP from VOC when they're both from the same data source
- Could lead to geographic inconsistencies in speciation (HAP reporting inconsistencies)

Conclusions

- We plan to combine HAP/CAP inventories for multipollutant modeling using an updated chemical mechanism in CMAQ
- Analyzed much of the 2002 NEI to determine extent to which HAP/CAP sources can be integrated
- Found a large amount of VOC mass will be using the “integrate” case, allowing us to maximize the use of the HAP inventory