



EPA's SPECIATE DATABASE AND ITS APPLICATIONS

DAVID MOBLEY¹, LEE BECK², MARC HOYOUX³, ADAM REFF¹ AND GOLAM SARWAR¹

¹US-EPA, OFFICE OF RESEARCH AND DEVELOPMENT, NATIONAL EXPOSURE RESEARCH LABORATORY

²US-EPA, OFFICE OF RESEARCH AND DEVELOPMENT, NATIONAL RISK MANAGEMENT RESEARCH LABORATORY

³US-EPA, OFFICE OF AIR AND RADIATION, OFFICE OF AIR QUALITY PLANNING AND STANDARDS

SPECIATE Database

What is SPECIATE?

- Database of speciated emissions profiles by source category
- Disaggregated into particulate matter (PM) and total organic gases (TOG)
- Species include compounds, elements and PM size fractions
- Housed in MS Access

Why Do We Need A Speciated Emissions Database?

- Modeling
 - Air quality modeling
 - Source-receptor modeling
 - Emissions characterization
- Searchable repository
- Tool for data processing
 - Can integrate with spreadsheets
 - Export to other programs (e.g., GIS)

Brief History

- Paper and computerized versions available in 1988 for EPA applications
- First electronic (CD) version distributed to the user community in 1993
- Speciate 3.2 posted to EPA's CHIEF website in November 2002
- Speciate 4.0 Posted to EPA's CHIEF website January 2007

Summary of Changes

SPECIATE 3.2	SPECIATE 4.0
1503 PM profiles	2865 PM profiles
565 gas profiles	1215 gas profiles
890 unique species	1902 unique species

Speciate 4.0

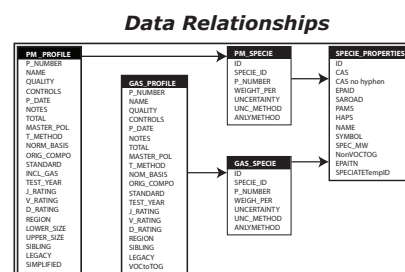
- Requires MS Access®
- Website also has documentation and other pertinent information
 - VOC-to-TOG conversion factors
 - SCC-Profile cross reference table
 - Protocol for expansion of the SPECIATE database
- Standard reports and queries are available



- Database available at <http://www.epa.gov/ttn/chief/software/speciate/index.html>

Example Fields in Access Tables

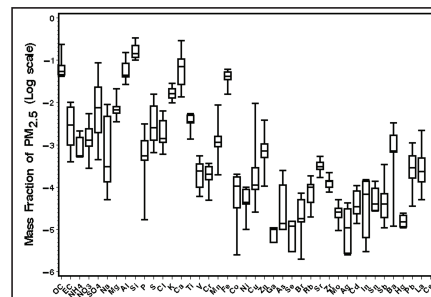
- Profile number and name
- Data quality rating
- Emission controls
- Test year, notes
- Analytical method
- Weight percent
- Uncertainty indicator



Composite Profiles

- Merger of multiple data sets for a source category
- 48 source categories
- A single number to be used for the source
- Addresses large disparate datasets (e.g., Unpaved Road Dust)

Speciate Profiles in Unpaved Road Dust Category



PM-Simplified Profiles

- 95 simplified profiles added to database (EC/OC, sulfate, nitrate, and PM-other)
- Used by air quality models

Source Classification Code-to-Profile Mapping

- Allows correlation of profiles to individual source categories
- Covers all Source Categories in EPA's 2002 National Emissions Inventory for VOC and PM emissions

Protocol for Database Expansion

- Full references are needed
- Electronic data preferred
- Send to beck.lee@epa.gov

Applications

Emission Inventory Enhancements

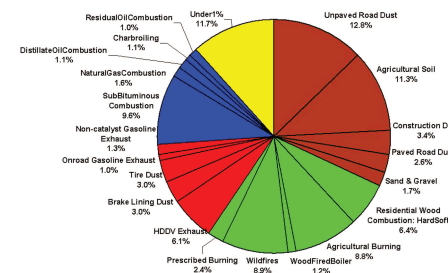
Changes in Emissions for the CB05 Mechanism in the Modeling Domain for July 1, 2001

VOC_SPECIES	SPECIATE_3.2 moles/sec	SPECIATE_4.0 moles/sec	Percent change %
ALD2	17,600	19,500	11
ALDX	8,300	8,200	-1
ETH	50,000	49,000	-2
ETHA	16,000	13,000	-19
ETOH	44,000	43,000	-2
FORM	37,000	38,000	3
IOL	40,000	40,000	0
ISOP	231,000	231,000	0
MEOH	110,400	113,000	2
OLE	68,000	70,000	3
PAR	736,000	720,000	-2
TERP	52,000	52,000	0
TOL	14,000	10,000	-29
XYL	10,000	7,000	-30
PM_SPECIES	gm/sec	gm/sec	
PEC	261,000	230,000	-12
PM_OTHER	1,833,000	1,973,000	8
PN03	5,800	13,000	124
POA	563,000	473,000	-16
PSO4	169,000	142,000	-16

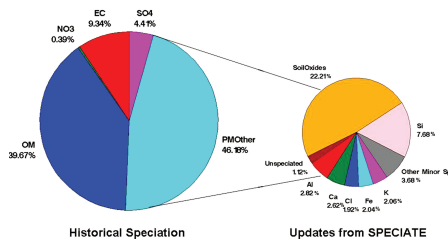
Source Receptor Modeling

- SPECIATE 4.0 has been integrated with the emission inventory to improve source apportionment and species characterization
- Improved species profiles lead to improved emission characterization for source-receptor modeling applications as shown below

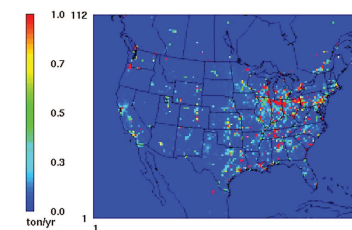
PM_{2.5} Emission by Types of Source Categories from SPECIATE



Speciation of National PM_{2.5} Emissions using Speciate Profiles

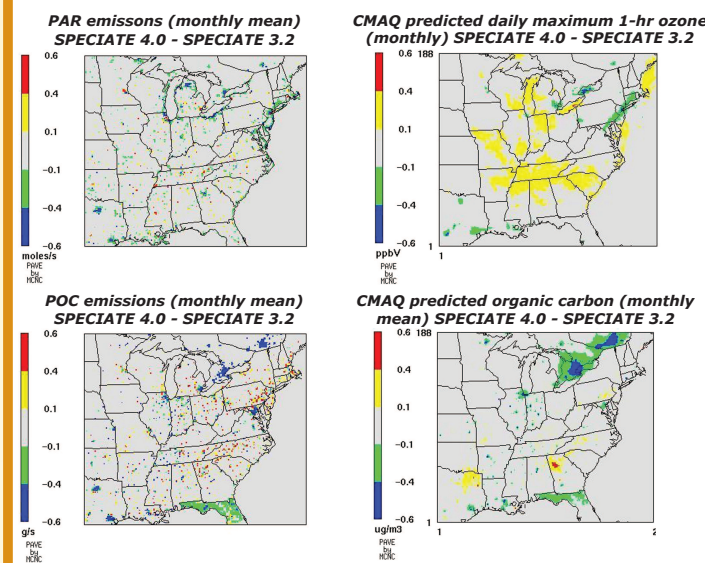


Spatial Distribution of Ni Emissions



Air Quality Modeling

- SPECIATE 4.0 has been integrated into the Emissions Modeling Platform for air quality modeling applications
- Emission species changes impact air quality modeling concentrations as shown below



Summary

- SPECIATE 4.0 represents a significant enhancement of the data available to characterize emissions by species and source category
- Air quality modeling and source-receptor modeling applications are improved using these enhanced speciation profiles
- Additional efforts are needed to capture new data from current testing
 - SPECIATE 4.1 to include Canadian data
 - SPECIATE 4.2 to update mobile source profiles
 - New profiles will be added in future revisions based on data submitted via the protocol for database expansion
- You can help by supplying data
 - Full references are needed
 - Electronic data preferred
 - Send to beck.lee@epa.gov

Disclaimer: Although this material has been reviewed and approved for presentation, any views expressed by the authors do not necessarily reflect the views of the US Environmental Protection Agency