



EPA's SPECIATE 4.4 Database: Development and Uses

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The SPECIATE Work Group

Introduction

- SPECIATE and its use
- SPECIATE 4.4 highlights
- Linking VOC profiles to SCC categories for the 2011 NEI modeling platform
- SPECIATE 4.5 and future plans

What is SPECIATE?

- A repository for speciated emissions profiles
- A searchable Microsoft Access database
- Profiles for three air pollution emission types:
 - Particulate Matter (PM)
 - Volatile Organic Compounds (VOCs)
 - Other Gases [Hg, NO/NO₂/HONO, semivolatile organic compounds (SVOCs)]
- Species include metals, ions, elements, organic and inorganic compounds
- PM profiles are size-segregated (PM₁₀, PM_{2.5})
- Profiles are rated for quality

SPECIATE is a collaboration involving:

- EPA's Office of Research and Development (ORD)
- EPA's Office of Air Quality Planning and Standards (OAQPS)
- EPA's Office of Transportation and Air Quality (OTAQ)
- The SPECIATE Workgroup

Why Do We Need SPECIATE?

DATA SOURCES → SPECIATE → DATA USERS

Peer-reviewed Literature

Source Testing of
Speciated Emissions

Primarily EPA Data



Input to Regulatory Models
2011 NEI Modeling Platform

- CMAQ
- MOVES
- SMOKE

Source Apportionment
Source Receptor Models
Air Toxics Inventories

Feedback on Data Needs



Uses of SPECIATE Data

IMPACT OF SPECIATED EMISSION PROFILES APPLIED TO THE NEI

- Analysis performed by SPECIATE Workgroup (**Simon et al.**, 2010)
- Compared emissions extracted directly from the NEI to NEI emissions adjusted using SPECIATE profiles
 - Included 96 HAPs from 12 source categories

Impact of Speciated Emission Profiles Applied to the NEI

- Identified many cases with large differences
 - For Mobile Sources, when adjusted:
 - Aromatic and aldehyde emissions were higher
 - MBTE and 2,2,4-trimethylpentane were lower
 - For Solvent Utilization, when adjusted:
 - Toluene, xylene and acetaldehyde emissions were higher
 - Benzene was lower

SPECIATE 4.4 Highlights

- Summary of New Profiles
 - 32 new PM profiles for a total of 3,600
 - 104 new Organic Gas profiles for a total of 1,879
 - 0 new Other Gases profiles for a total of 249
 - 2,346 unique species
- Sources of New Profiles
 - Organic Gases - Oil and Gas Fugitive Sources
 - Organic Gases - Gasoline Vehicle Exhaust
 - Organic Gases - Dairy Farms
 - PM - the Kansas City light vehicle study
 - PM - Outdoor Wood Boiler aerosol emissions
 - PM - Aircraft Exhaust

SPECIATE 4.4 Highlights (cont.)

Supports two OTAQ efforts

- The Tier 3 Vehicle Emission and Fuel Standards Program for the 2017 model year
 - Provides readily accessible speciation data
 - Increases the transparency of the rulemaking process
- Release of MOVES2014
 - Required for state implementation plan (SIP) development
 - Directly incorporates speciation profiles

Linking VOC Profiles to SCCs for the 2011 NEI Modeling Platform

- SPECIATE Background
 - Every VOC profile assigned by its SCC to a source category
 - The SCC-to-SPECIATE cross-reference table accounts for over 80% of national VOC and PM emissions in the National Emissions Inventory (NEI)
 - But, how well are these cross referenced?

Linking VOC Profiles to SCCs for the 2011 NEI Modeling Platform

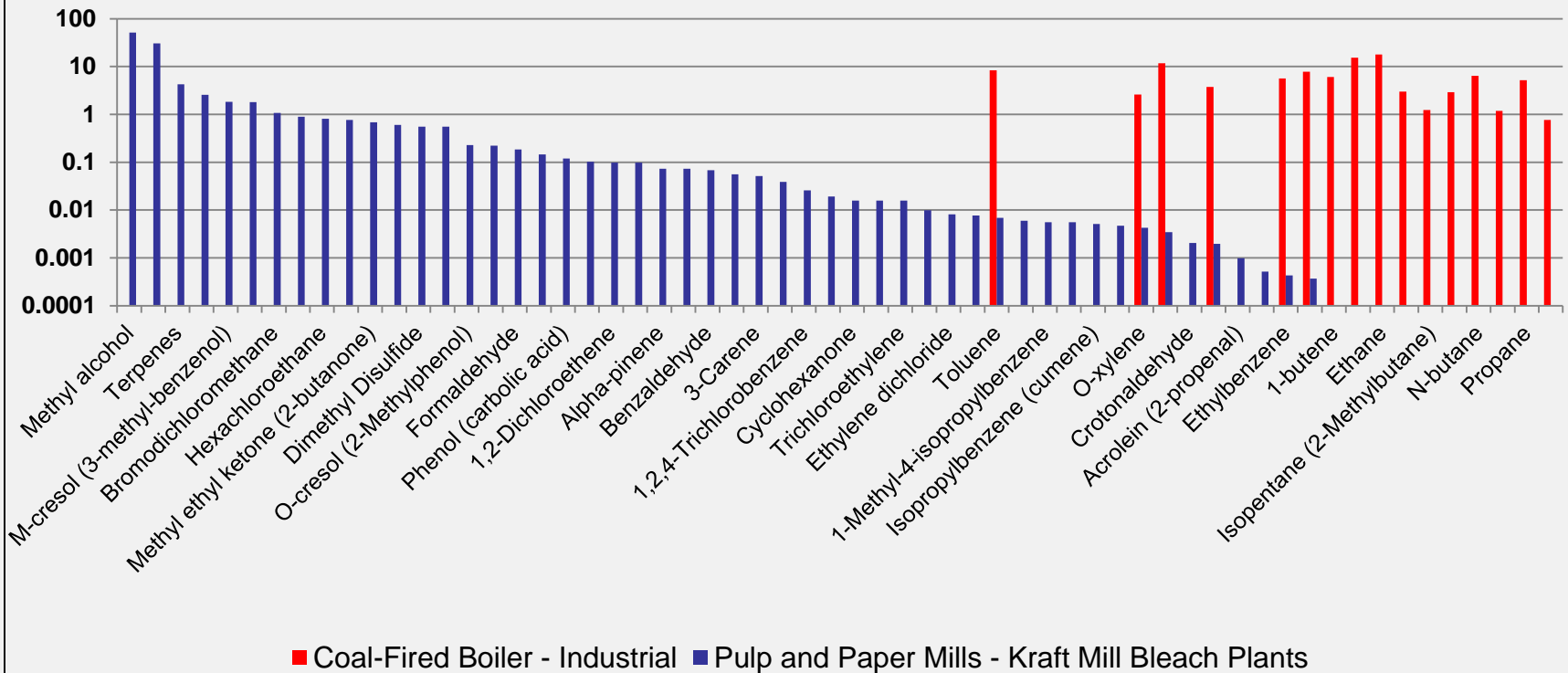
- Abhinav Sehgal, EPA Student Volunteer, Summer of 2013
- Project Goal
 - Review VOC emission profiles applied to SCC categories that are for the largest sources of VOCs
 - Identify SCC categories with potentially better profiles

Analysis of Pulp and Paper Profiles

- Abhinav found that:
 - Over 200 Pulp and Paper profile assignments for source categories are linked to generic profiles
 - Potentially better profile matches exist for only 21 sources
 - The eight largest of these matches are linked to profile 1185: *Coal Fired Boiler – Industrial*

Comparison of Old and New Profiles for One SCC Category

Chemical Composition: Coal-Fired Boiler - Industrial vs. Pulp and Paper Mills - Kraft Mill Bleach Plants



Industry Sector VOC Profiles for the 2011 NEI Modeling Platform

- Many Pulp and Paper SCCs
 - Have no appropriate available profile
 - Use the default speciation profile based on all emission sources contained in SPECIATE 3.2
 - The emissions inventory would be improved by using more appropriate profiles
- Overall, the 2011 NEI Platform has over 150 kT of volatile organic gases speciated with the default profile

Industry Sector VOC Profiles for the 2011 NEI Modeling Platform

- Pulp and Paper
 - Alexis Zubrow of EPA and Environ
 - Part of 2011 NEI Modeling Platform effort
 - Developed and applied a composite source profiles for the Pulp and Paper sector from SPECIATE emissions profiles
 - Improved the emissions profiles linked to SCCs

Industry Sector VOC Profiles for the 2011 NEI Modeling Platform

- Pulp and Paper –
Summary of Improvements

Industry Sector VOC Profiles for the 2011 NEI Modeling Platform

- Similar Exercise Completed for
the Chemical Manufacturing
Sector
- Summary of Improvements

SPECIATE 4.5 To Date

- Added 54 speciated PM emission profiles
 - Cook stoves, garbage burning, brick kilns, wood stoves, fireplaces, prescribed burning, coal combustion and welding fumes
- Added nine speciated TOG profiles
 - Oil and gas production, prescribed burning, petroleum refining, dairy operations and poultry production.
- Added 91 chemical species
 - Emission sources included woodstoves and fireplaces.

Current Goals

- Utilize resources provided by ORD and Region 8 to increase SPECIATE's coverage of oil and gas emissions profiles
- Improve capture of metadata
 - Sampling and analysis methods
 - Subjective profile quality ratings
- Link new profiles to Source Classification Codes (SCCs) in the NEI
- Assign species to photochemical reactivity classes

Workgroup Committees

- The Black Carbon (BC) Committee
 - Investigating analytical methods to measure BC, whether scientifically meritorious BC data to be incorporated into speciation profiles
- The Maximum Incremental Reactivity (MIR) Committee
 - Investigating whether MIR values should be incorporated into SPECIATE as a new data field
- The Secondary Organic Aerosols (SOA) Committee
 - Evaluating SOA and brown carbon issues

Other Opportunities

- Sector-based composite source profiles
- Unspeciated organic emissions from combustion
 - Potential influence on inventories of secondary organic aerosols (SOA)
 - Key source sectors - biomass burning, wood burning, on-road and off-road vehicles
- Global climate (methane and BC)
 - Many partners looking for support
 - Potential addition of EC and OC to future NEIs
 - Methane as a criteria air pollutant subject to the NAAQS?

Questions/Comments/Suggestions

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