EPA's SPECIATE 4.4 Database: Development and Uses

Michael Kosusko, EPA/ORD/NRMRL
Prakash Bhave, ICIMOD
Alexis Zubrow, EPA/OAR/OAQPS
Ying Hsu, Jonathan Dorn, Frank Divita, Abt Associates
The SPECIATE Work Group

Office of Research and Development
National Risk Management Research Laboratory, Air Pollution Prevention and Control Division

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Introduction

- SPECIATE and its use
- SPECIATE 4.4 highlights
- Linking Total Organic Gas (TOG) profiles to Source Classification Codes (SCCs) for the 2011 National Emission Inventory (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)
  - Total Organic Gases (TOGs)
  - Other Gases [Hg, NO/NO_2/HONO, semivolatile organic compounds (SVOCs)]
- Species include metals, ions, elements, organic and inorganic compounds
- PM profiles are size-segregated (PM_{10}, $PM_{2.5}$)
- Profiles are rated for quality

SPECIATE is a co-funded by:

- 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)

who are informally represented on 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

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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 applying SPECIATE profiles
  - Included 96 hazardous air pollutants (HAPs) from 12 source categories

Impact of Speciated Emission Profiles Applied to the NEI

- Identified many cases with large differences
  - For Mobile Sources, when speciated:
    - Aromatic and aldehyde emissions were higher
    - MBTE and 2,2,4-trimethylpentane were lower
  - For Solvent Utilization, when speciated:
    - 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 TOG 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
  - TOG - Oil and Gas Fugitive Sources
  - TOG - Gasoline Vehicle Exhaust
  - TOG - Dairy Farms
  - PM - the Kansas City light vehicle study
  - PM - Outdoor Wood Boiler aerosol emissions
  - PM - Aircraft Exhaust

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

- SPECIATE Background
  - Every TOG 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 NEI
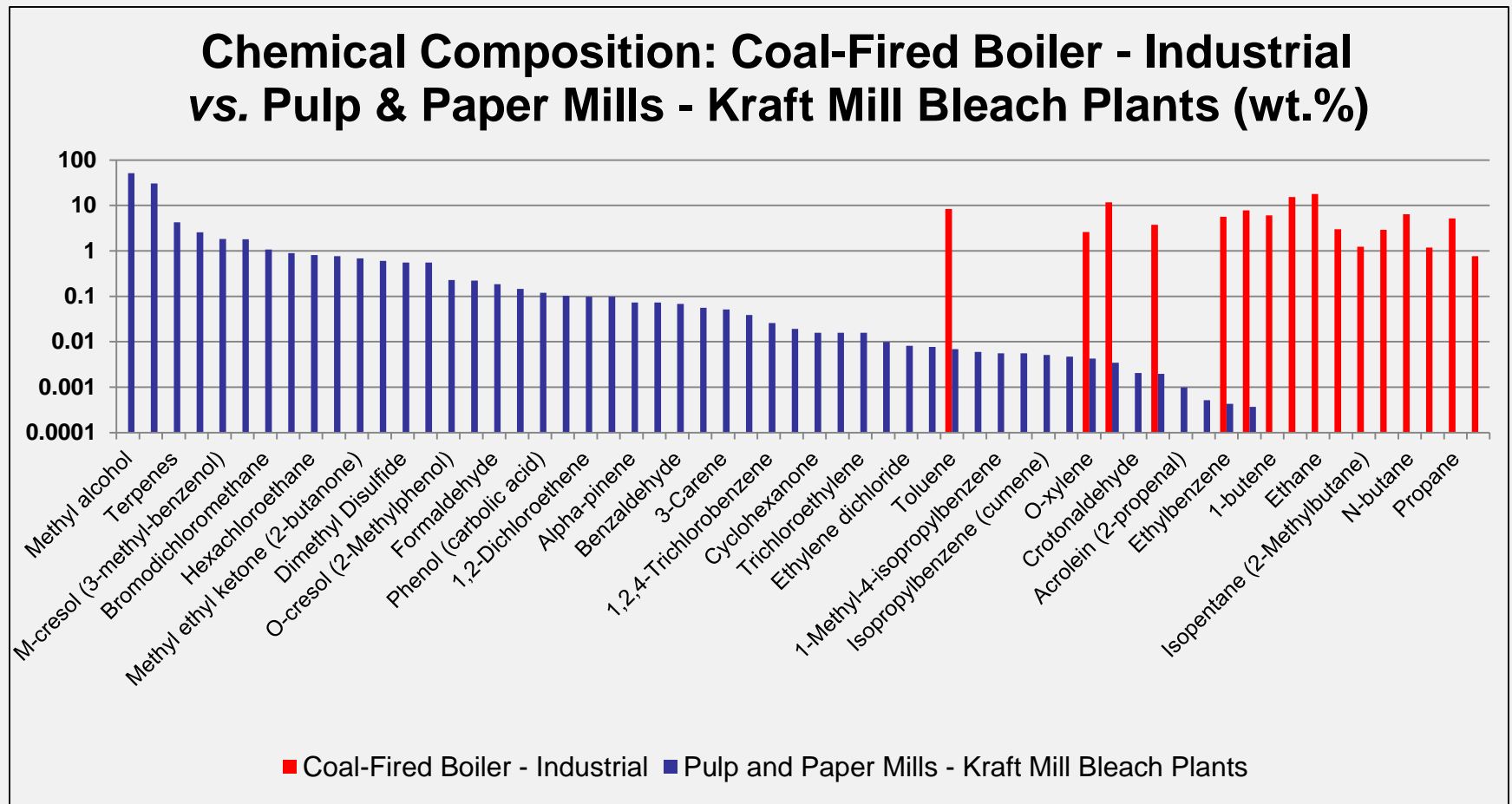 - But, how well are these cross referenced?

Linking VOC Profiles to SCCs for the 2008 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*
  - Profile 1185 linked 43 of 144 kTpy from Pulp and Paper

Comparison of Old and New Profiles

Chemical Composition: Coal-Fired Boiler - Industrial *vs.* Pulp & Paper Mills - Kraft Mill Bleach Plants (wt.%)

Legend: ■ Coal-Fired Boiler - Industrial ■ Pulp and Paper Mills - Kraft Mill Bleach Plants

Industry Sector TOG Profiles from the 2008 NEI

- 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
- The 2008 NEI has well over 500 kTpy of volatile organic gases speciated with the SPECIATE 3.2 default profile (0000)

Industry Sector TOG Profiles for the 2011 NEI Modeling Platform

- Pulp and Paper
  - Alexis Zubrow, EPA, supported by 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
  - Composite profiles added to SPECIATE 4.5
  - Improved the emissions profiles linked to SCCs

Industry Sector TOG Profiles for the 2011 NEI Modeling Platform

- Pulp and Paper
  - 97 of 121 kTpy assigned to profiles 0000 and 1185 in the 2011 NEI
- Summary of Improvements

Industry Sector VOC Profiles for the 2011 NEI Modeling Platform

- Similar Exercise Completed for the Chemical Manufacturing Sector
  - 20 of 90 kTpy assigned to profile 0000 in the 2011 NEI
- Summary of Improvements

SPECIATE 4.5 To Date

- Added 146 speciated PM emission profiles
  - Cook stoves, garbage burning, brick kilns, biomass and coal combustion, wood stoves, fireplaces, prescribed burning and welding fumes
- Added 184 speciated TOG profiles
  - Oil and gas production, petroleum refining, mobile sources, residential wood combustion, prescribed burning, agricultural operations
- Added more than 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 SCCs in the NEI

- Assign species to photochemical reactivity classes

Workgroup Committees

- The Black Carbon (BC) Committee
  - Investigating analytical methods to measure BC and whether BC data can be incorporated into speciation profiles

- The Maximum Incremental Reactivity (MIR) Committee
  - MIR values are being 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 elemental and organic carbon (EC and OC) to future NEIs
  - Methane as a criteria air pollutant subject to the NAAQS?

Questions/Comments/Suggestions

Please contact:

Michael Kosusko, US EPA

(919) 541-2734

Kosusko.Mike@epa.gov