EPA Science Training Webinar: SPECIATE Database

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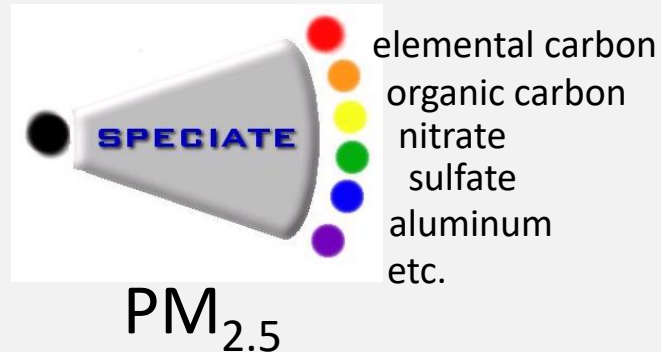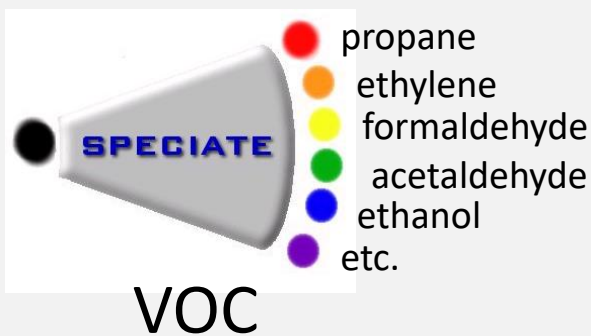
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What we will cover

- What is SPECIATE, who works on it

- Uses/Importance of SPECIATE

- Database and Browser

What is SPECIATE?

EPA's repository of source-based speciation profiles that provides the chemical composition of organic gas such as volatile organic compounds (VOC), particulate matter (PM) and other pollutants (such as mercury)

- Example Sources: wildfires, household product usage, oil and gas operations, charbroiling and frying, road dust

propane
ethylene
formaldehyde
acetaldehyde
ethanol
etc.

VOC

elemental carbon
organic carbon
nitrate
sulfate
aluminum
etc.

PM$_{2.5}$

Elemental Hg
Divalent Hg
Particulate Hg

Mercury

Purpose of SPECIATE

- To organize and make available scientifically sound organic gas, PM and other pollutants' speciation profile data

  - Data can be from EPA, state agencies, peer-reviewed literature and other relevant data sources

  - SPECIATE also provides additional metadata elements useful to the users of speciation data

  - Example data provided:

    - Emission source category (e.g., wildfires, oil and gas production)

    - Weight percent of PM/VOC chemical species

    - Test methods, year, reference(s), etc.

    - Reference(s)

SPECIATE is a cross-office, collaborative and ongoing effort:
EPA ORD and OAR (OAQPS & OTAQ[1])

Co-leads: George Pouliot, ORD and Art Diem, OAQPS

SPECIATE WORKGROUP MEMBERSHIP		
NAME	**EPA OFFICE**	**EXPERTISE/SPECIALIZATION**
Souad Benromdhane	OAR[2]/OAQPS	Health Benefits of Air Quality Management
Casey Bray	OAR/OAQPS	Emission Source Speciation
Art Diem	OAR/OAQPS	Co-lead, HAPs and Air Toxics
Justine Geidosch	OAR/OTAQ	Mobile Source Emissions
Ingrid George	ORD	Emission Source Testing and Black Carbon
Michael Hays	ORD	Emission Source Testing
Brooke Hemming	ORD/NCEA	Climate Change and Black Carbon
Amara Holder	ORD	Emission Source Testing and Black Carbon
George Pouliot	ORD	Co-Lead, Emissions Modeling (Inventories and Platforms)
Ben Murphy	ORD	Secondary Organic Aerosol Modeling
Libby Nessley	ORD	QA Manager
Havala Pye	ORD	Secondary Organic Aerosol Modeling
Karl Seltzer	ORD	Secondary Organic Aerosol Modeling, Volatile Chemical Products
Venkatesh Rao	OAR/OAQPS	Biomass Burning and Black Carbon Inventory
Heather Simon	OAR/OAQPS	Air Quality Modeling
Tiffany Yelverton	ORD	Air Pollution Control, Combustion, and Black Carbon

Team meets twice a month to discuss profile priorities, data availability, resource planning and contract management

[1] OTAQ: Office of Transportation and Air Quality   [2] OAR: Office of Air and Radiation

Primary Uses of SPECIATE: Air Quality Modeling

- Regulatory model applications
  - Air quality standards
  - Sector & transport, rules
- Research model development
  - Secondary organic aerosol treatment
  - Chemical mechanisms
  - Specific sector analysis: Volatile chemical products, Oil and gas
- Assessments and health studies (e.g., National Air Toxics Assessment)

Other Key Uses

- Estimate black carbon (elemental carbon ~ black carbon) and organic carbon for use in carbon emission assessments and inventories

  - SPECIATE is the basis for all black carbon (BC) input to the global climate models used to forecast future climate scenarios (Bond et al. 2004)

  - EPA's Black Carbon Report to Congress

  - Arctic deposition study

- Source apportionment

- Estimate air toxics emissions

- Used in international community for addressing PM and VOC speciation needs

Who cares and why?

- SPECIATE is a ***workhorse*** for Air Quality Models
  - Domestic and international

- Over a thousand research and policy planning institutes have published citing SPECIATE

- States use SPECIATE in their air quality models for their State Implementation Plans (SIPs)
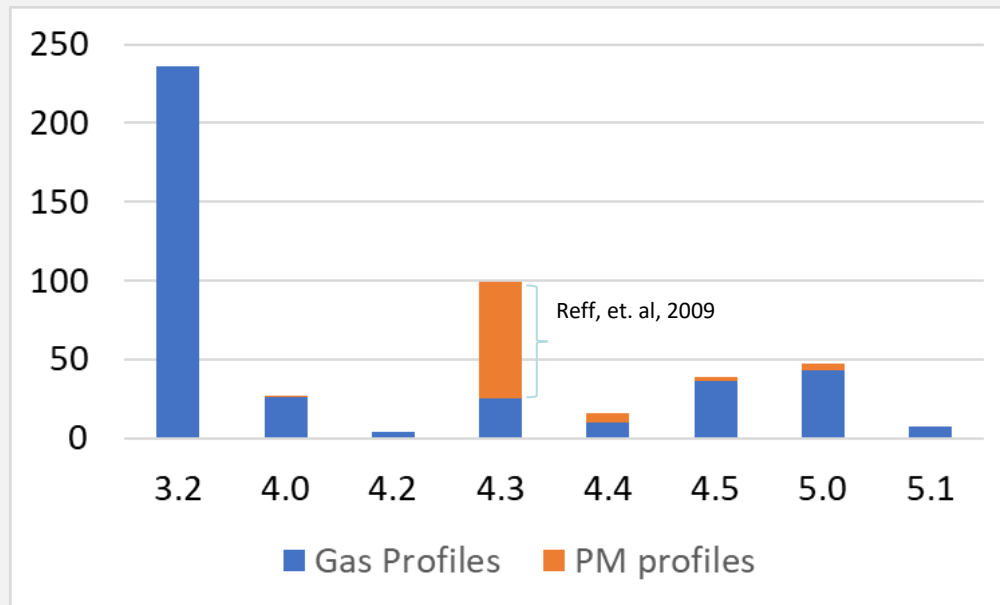
SPECIATE 5.1: Expansion of the Database
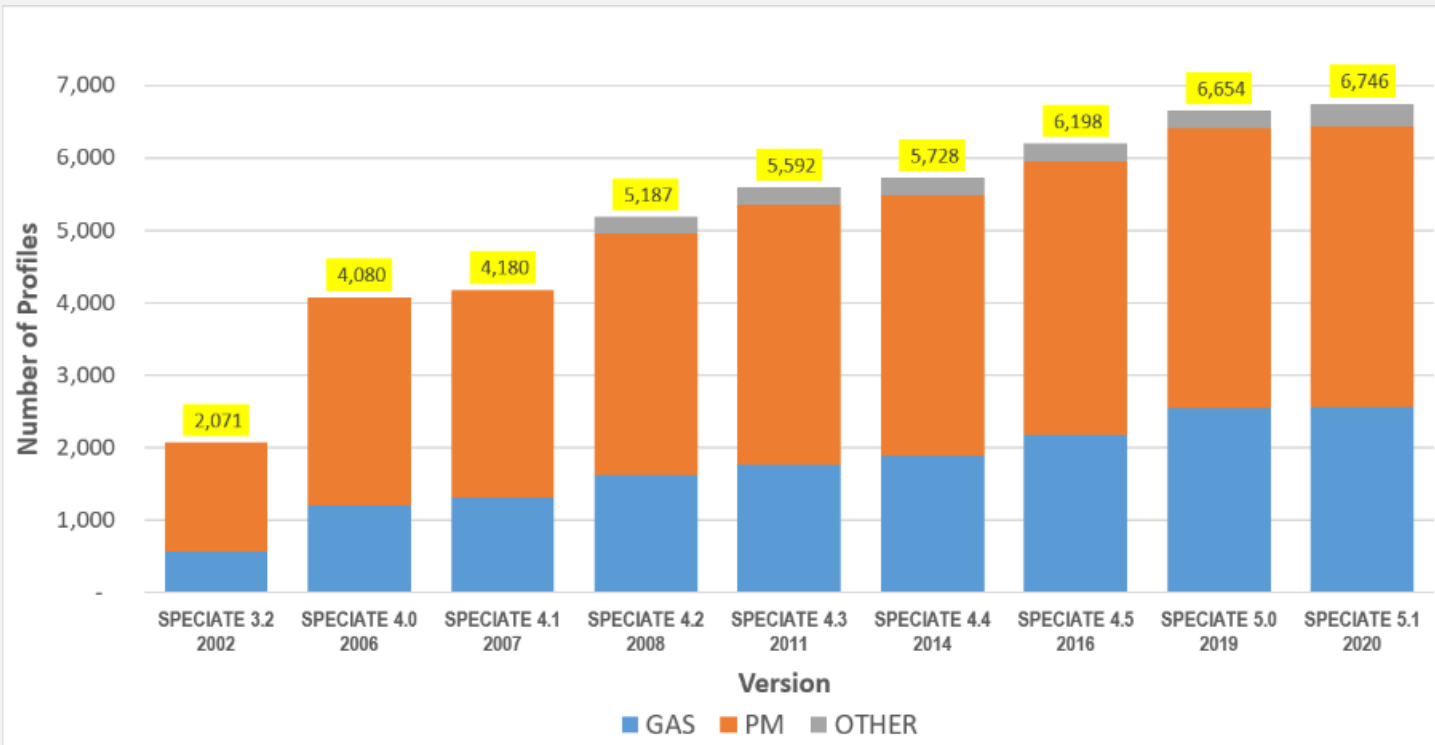
SPECIATE 5.1
6,746 profiles
# of Profiles
Added:
16 Gas,
18 PM$_{2.5}$
58 mercury

Each version is a cumulative update of the previous version

Profiles used in Modeling (2017) by SPECIATE version

Reff, et. al, 2009

Gas Profiles   PM profiles

- Thousands of National Emissions Inventory (NEI) source categories are mapped to a few hundred profiles
  - 475 profiles used in the platform (387 VOC; 88 $PM_{2.5}$)
  - Most are still from older versions of SPECIATE; (SPECIATE 3.2 released in 2002)

Adding data to SPECIATE

- Systematic process
- Starts at tracking the literature and other sources of available data
- Analyzing the data
- Developing profiles
- Review and Quality Score
- Enter into the database
- QA the database
- State Example: Oil and gas exploration and production speciation data for a specific basin

Flow Chart

Evaluating the Addition of Speciation Profiles to the SPECIATE Database
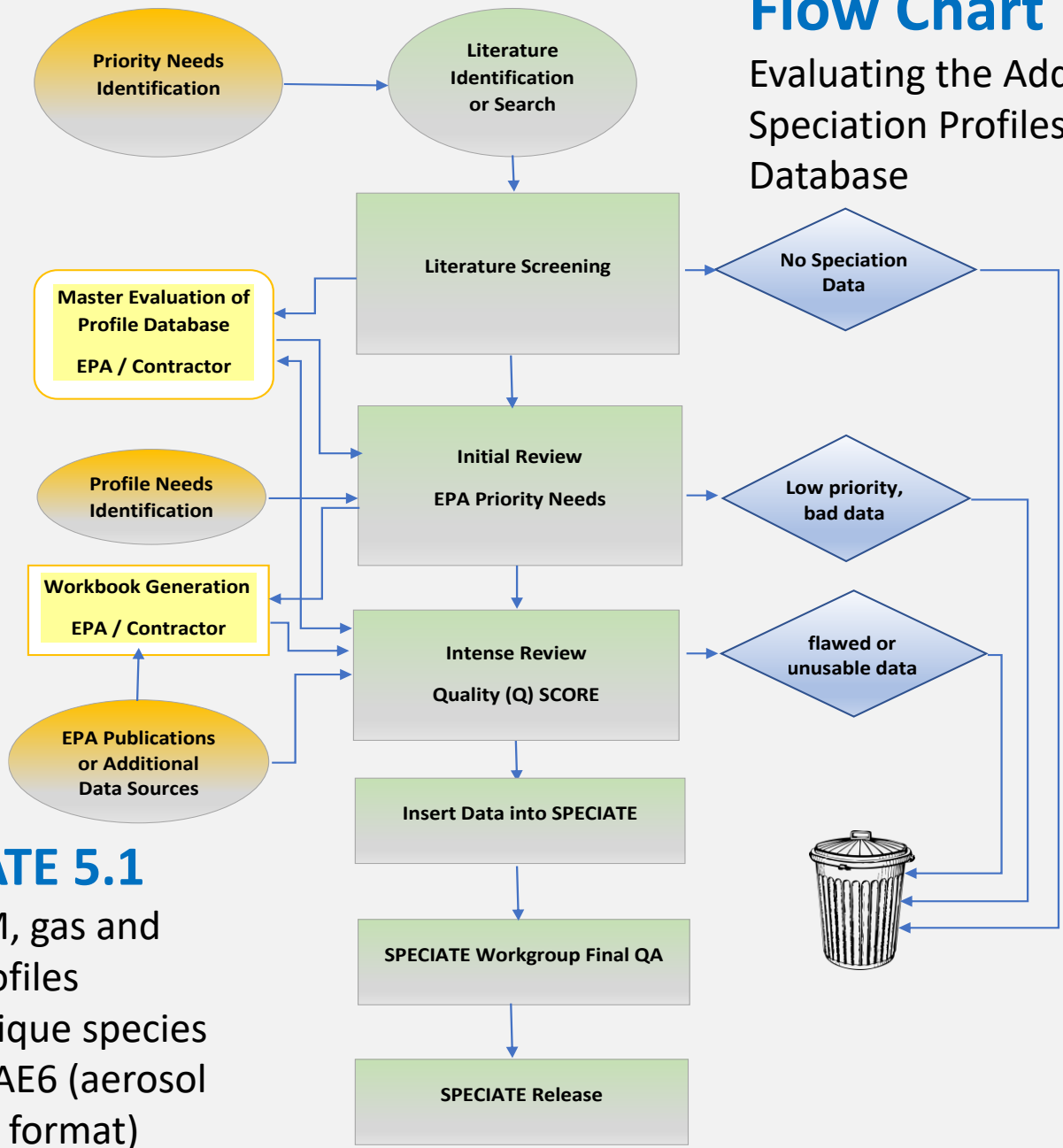
SPECIATE 5.1

6,746 PM, gas and other profiles
2,814 unique species
198 PM-AE6 (aerosol module6 format)

Systematic approach: Priority needs

- *An assessment of important SPECIATE profiles in the EPA emissions modeling platform and current data gaps*, by Casey D. Bray, Madeleine Strum, Heather Simon, Lee Riddick, Mike Kosusko, Marc Menetrez, Michael Hays, Venkatesh Rao, Atmospheric Environment, Volume 207, 15 June 2019, Pages 93-104, https://doi.org/10.1016/j.atmosenv.2019.03.013

  - Residential Wood Combustion
  - Nonroad
  - Fires (wild, prescribed, agricultural)
  - Oil and gas

  ORD research program/ OAQPS resources helping to fill some of the gaps. States may also have data!

- Appropriate source matching between literature and NEI
  - Thousands of source classification codes (SCCs) in the NEI are mapped to a few hundred profiles

A major step in putting profiles in SPECIATE: The QSCORE review/ranking process

- The Quality Criteria Factors (QSCORE) provide an evaluation framework

  The QSCORE evaluation is based on a series of questions with points assigned

  An ideal QSCORE would have 30 (data from Measurements) or 29 (data from other Methods)

  The ranks associated with the evaluation score points are as follows:
  - 22-30 = excellent
  - 16-21 = good
  - 8-15 = fair
  - <7 = poor

- Each numerical ranking (QSCORE) and description (excellent, good, fair, poor) are added to the SPECIATE Database
- EPA's cross-office SPECIATE Workgroup develops the QSCORE for every profile via team discussions

Guidelines for data developers

- Created documentation to help guide researchers/data developers develop data (voluntarily) and publications that will be useful to SPECIATE, including:
  - 'How-To' document
  - Template for data developers to use when voluntarily developing profiles
  - Email for questions/comments/collaboration requests: **SPECIATE_WG@EPA.GOV**

New Profiles – SPECIATE 5.0 (July 2019) and SPECIATE 5.1 (July 2020)

- Added Profiles
  - 370 new GAS profiles in 5.0 plus 16 in 5.1 for a total of 2,561 (GAS, GAS-VBS)
  - 86 new PM profiles in 5.0 plus 17 in 5.1 for a total of 3,878 (PM, PM-AE6, PM-SIMPLIFIED, PM-VBS (Volatility Basis Set))
  - 58 new mercury profiles in 5.1 for a total of 307 "Other" profiles
  - Of the above we have a total of 6 PM-VBS and 4 GAS-VBS profiles
- Added Profiles cover the following:

Gas (TOG - total organic gasses)
- Sugar cane burning
- Consumer products (multiple)
- Corrected heavy duty diesel
- Oil and gas (multiple)

PM (PM2.5)
- Wildfire
- Sugar cane burning
- Natural gas combustion
- Aircraft

Mercury
- Codified existing profiles for coal combustion and other sources from the UN's Global Atmospheric Mercury Assessment Programme
- New for geothermal power & cement kilns

VOC/TOG Terminology

Methane, ethane, acetone
Numerous CFCs and HCFCs
Many other "exempt" compounds

VOC

TOG
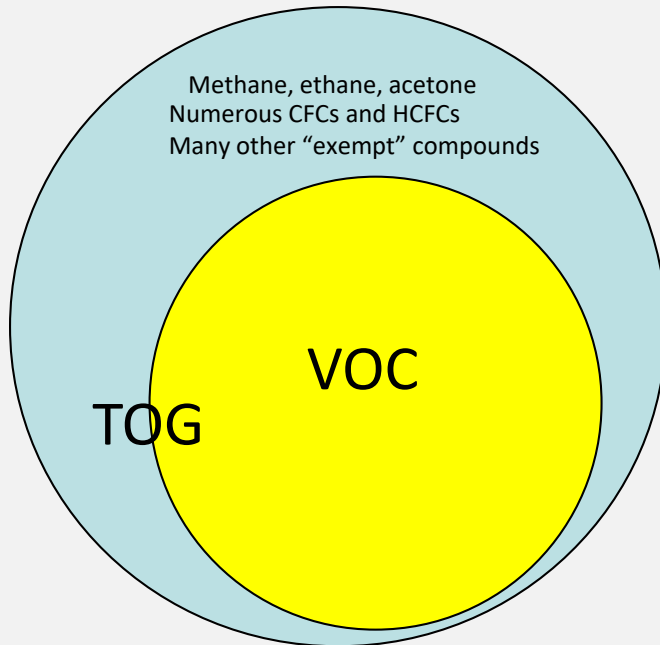
- Gas Profiles in SPECIATE can be based on VOC or TOG (see MASTER_POL field)
- Inventories have VOC (regulatory definition)
- TOG is "Total Organic Gases"
- TOG includes low reactivity and low volatility (low vapor pressure)
- TOG profiles have a factor that allow you to convert VOC to TOG

o **Total Organic Gases (TOG)** means "compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate."

VOC Exemption Information

- Electronic Code of Federal Register where the VOC information is available under Title 40 → Chapter I → Subchapter C → Part 51 → Subpart F → §51.100

- Volatile organic compounds (VOC) means any compound of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate, which participates in atmospheric photochemical reactions

- VOC Exempt compounds which have been determined to have negligible photochemical reactivity include but not limited to:
  - Methane, ethane, methylene chloride (dichloromethane),1,1,1-trichloroethane (methyl chloroform), … , certain classes of perfluorocarbon compounds

Converting VOC to TOG

- Ideally, when modeling you want emissions of TOG so you get all the species, but inventories give you VOC

- TOG profiles have a factor that allow you to convert VOC to TOG, called TOG_to_VOC ratio ≥ 1.0

- Already computed in the Database using this formula

    TOG to VOC ratio =

    (sum of profile weight percents)/(sum of VOC percent)

- Sum of profile weight percents is usually 100%

Example TOG Speciation Profile
(selected fields from the Query "View Gas Profiles")

PROFILE_CODE	PROFILE_NAME	CONTROLS	PROFILE_DATE	TOTAL	VERSION	VOC_to_TOG	SPECIES_ID	SPECIES_NAME	WEIGHT_PERCENT	VOC
0051	Flares - Natural Gas	Uncontrolled	05-Jan-89	100	3.2	2	438	Ethane	30	
0051	Flares - Natural Gas	Uncontrolled	05-Jan-89	100	3.2	2	465	Formaldehyde	20	YES
0051	Flares - Natural Gas	Uncontrolled	05-Jan-89	100	3.2	2	529	Methane	20	
0051	Flares - Natural Gas	Uncontrolled	05-Jan-89	100	3.2	2	671	Propane	30	YES

Assume you have 100 lb VOC from Flare – How much propane?

Mass of Propane = 100 lb VOC x (30/100) [lb propane/lb TOG]   x [2 lb TOG /1 lb VOC]
                = 60 lb

Browser to view and access data

- QLIK-based Browser App has been developed and is now available for all interested parties

  - Users can search for profiles by any of the fields associated with a profile or the species

  - Can sort by weight percent

  - New species names field (added in SPECIATE 5.1) has more synonyms so should be easier to find compounds

  - Can also use CAS or the DSSTX number (used by Computational Toxicology)

  - Users can visualize/compare profiles

Contacts

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www.epa.gov/air-emissions-modeling/speciate

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