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What's New in SPECIATE 5.2?

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SPECIATE

Outline

- What is SPECIATE, who works on it
- Uses/Importance of SPECIATE
- Updates for Version 5.2
- Speciate Browser

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What is SPECIATE?

EPA's repository of emissions 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)

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

SPECIATE WORKGROUP MEMBERSHIP		
NAME	EPA OFFICE	EXPERTISE/SPECIALIZATION
Souad Benromdhane	OAR/OAQPS	Health Benefits of Air Quality Management
Rich Cook	OAR/OTAQ	Mobile Source Emissions
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
Ben Murphy	ORD	Secondary Organic Aerosol Modeling
Casey Myers	OAR/OAQPS	Emission Source Speciation
Libby Nessley	ORD	QA Manager
George Pouliot	ORD	Co-Lead, Emissions Modeling (Inventories and Platforms)
Havala Pye	ORD	Secondary Organic Aerosol Modeling
Karl Seltzer	OAR/OAQPS	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

OTAQ: Office of Transportation and Air Quality OAR: Office of Air and Radiation

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SPECIATE

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 aka OAQPS Air Toxics Data Updates)

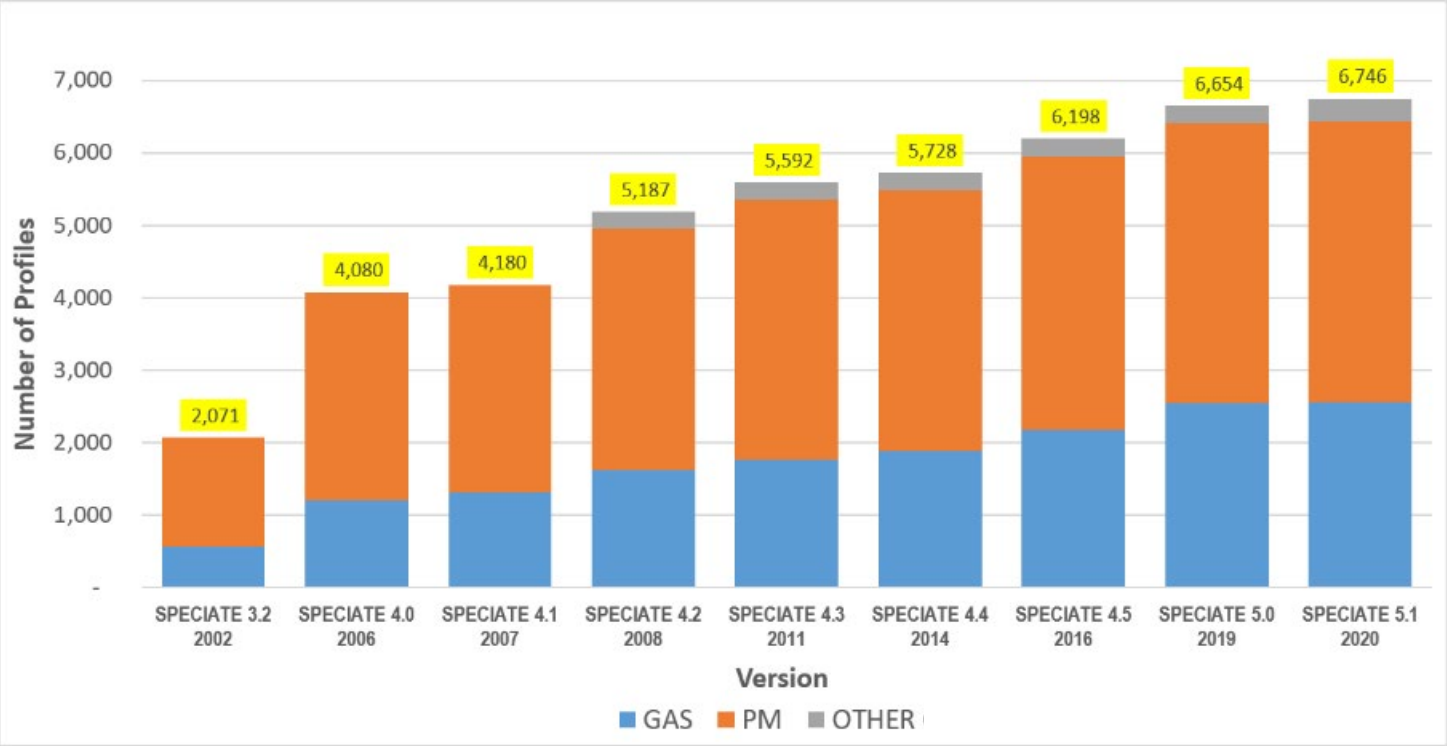
Other Key Uses

- 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)

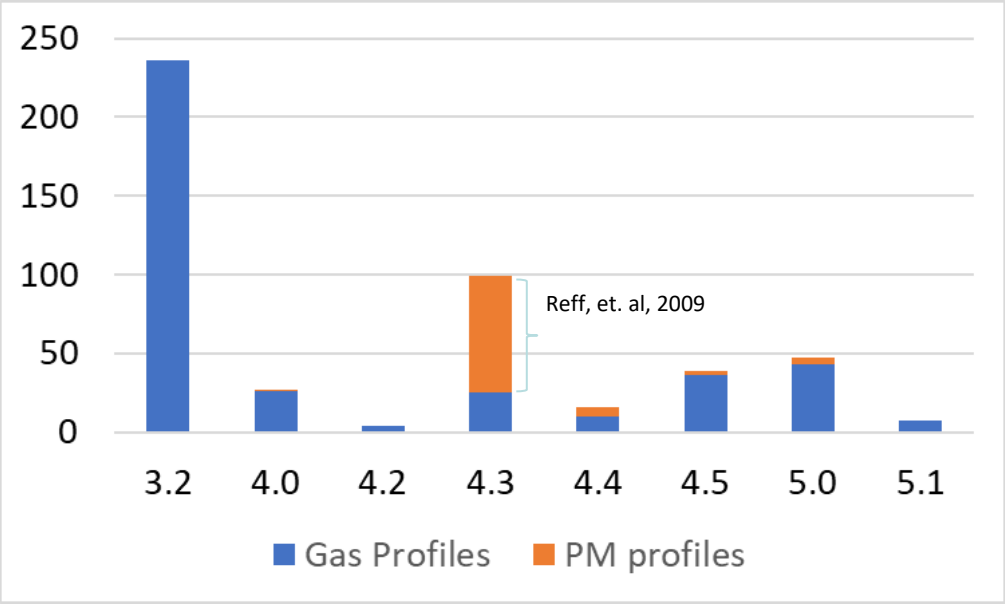
SPECIATE 5.1: Expansion of the Database



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 platform) by SPECIATE version



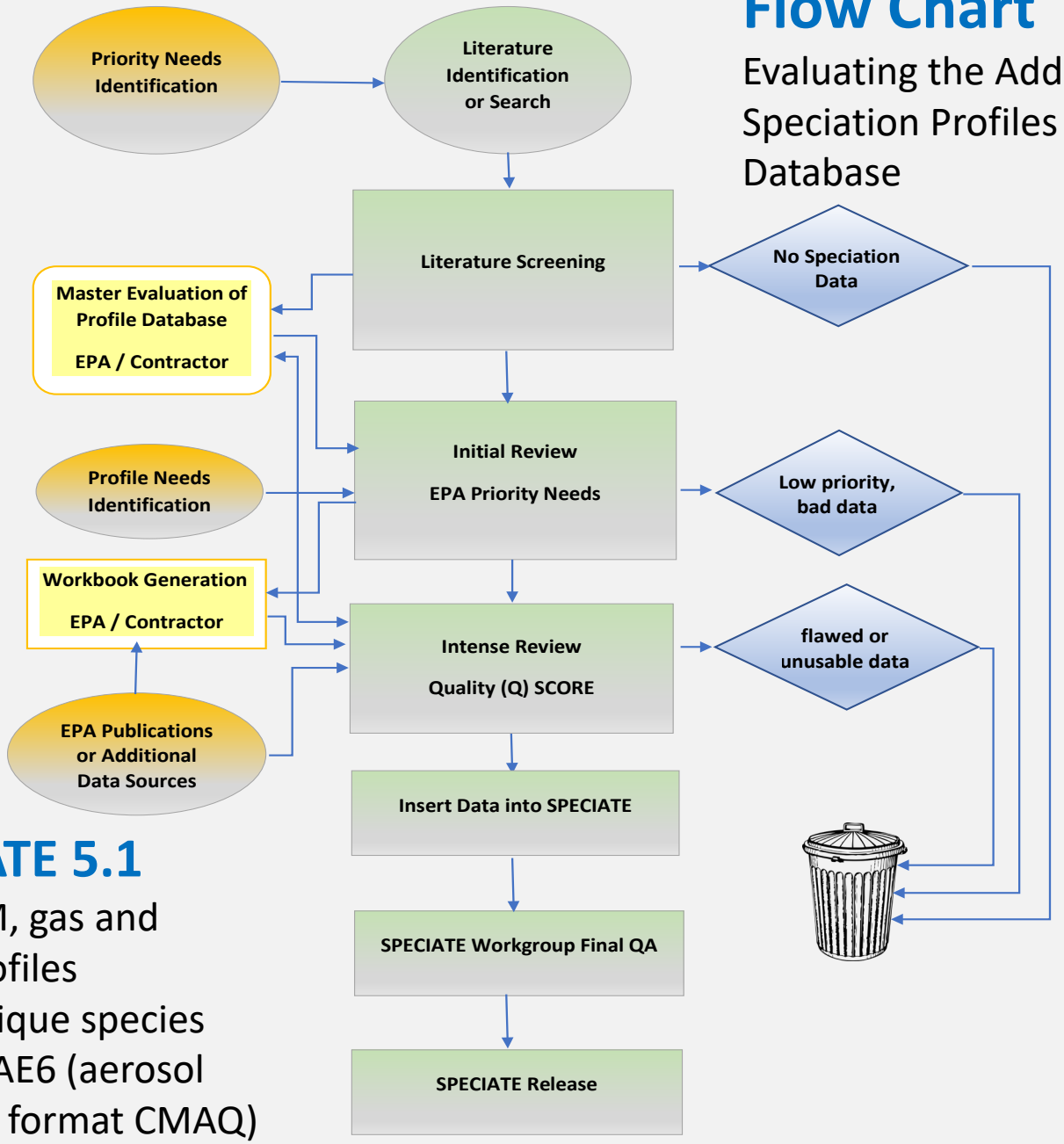
- Thousands of National Emissions Inventory (NEI) source categories are mapped to a few hundred profiles
  - 475 profiles used in the platform (387 VOC; 88 $PM_{2.5}$)
  - Most are still from older versions of SPECIATE; (SPECIATE 3.2 released in 2002)

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 the data 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



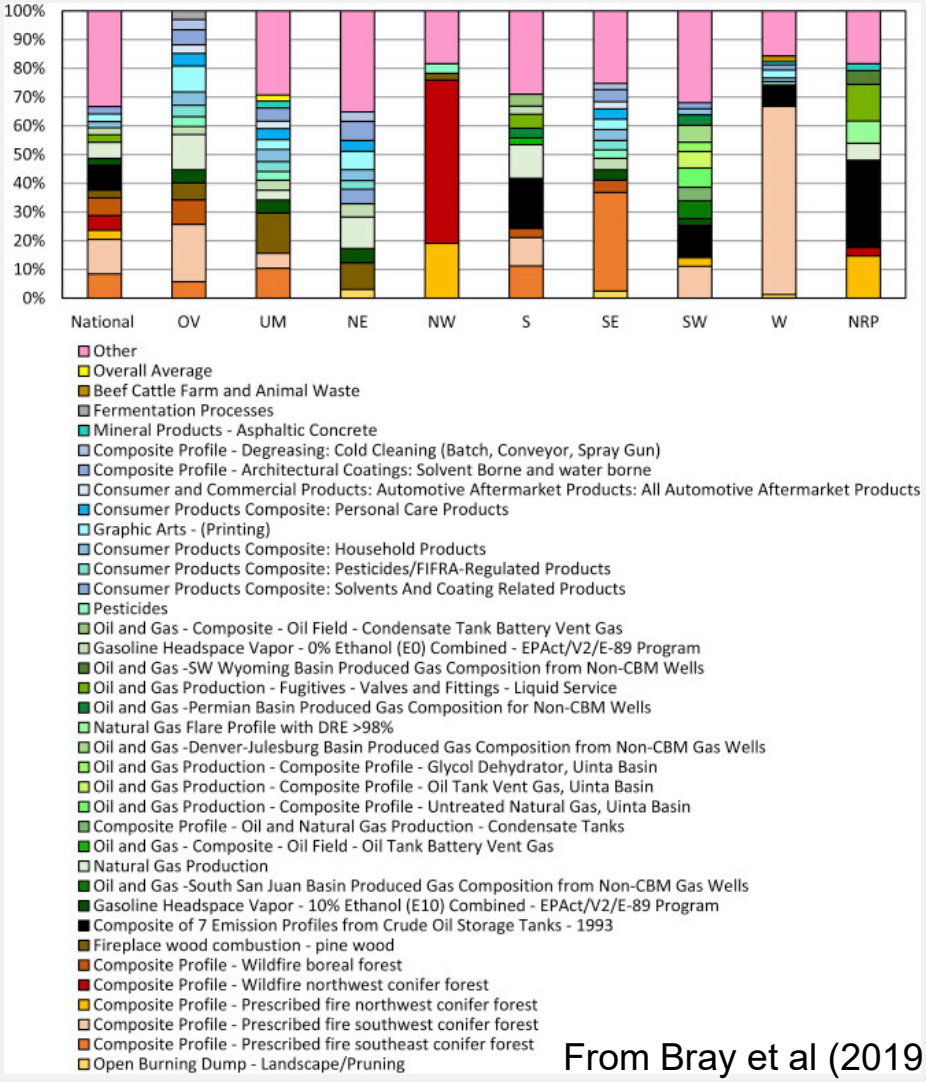
SPECIATE 5.1

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

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!



From Bray et al (2019)

Percent of emitted mass assigned to each VOC profile on a national scale and broken out by region

2014 modeling platform

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**
- **https://www.epa.gov/air-emissions-modeling/guide-data-developers**

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

Gas profiles can be used to calculate the mass emitted of a species of interest

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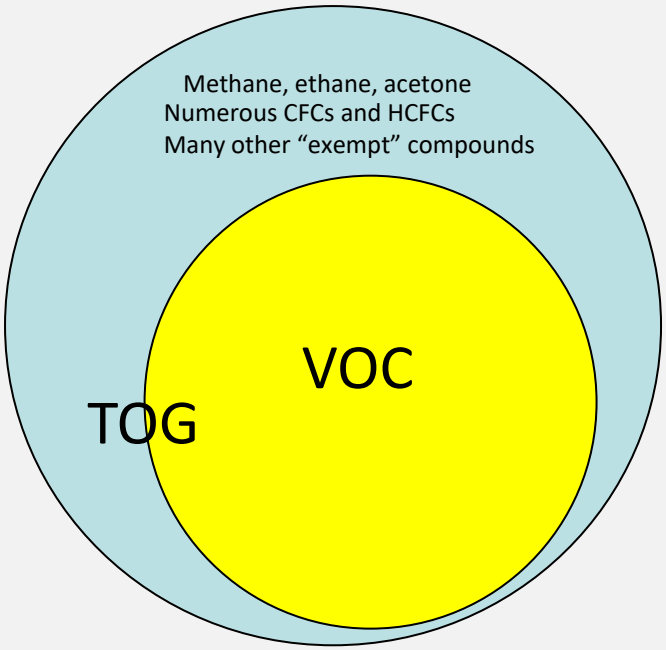
VOC/TOG Terminology



- Gas Profiles in SPECIATE can be based on VOC or TOG
- 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 can be used 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 (with 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

- Emissions of TOG are needed for air quality modeling since it includes all the species, but inventories only give VOC or something similar
- TOG profiles have a factor that can be used 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%

Updates for Version 5.2

- New Profiles in 5.2
  - Volatile chemical products profiles for “solvents” related emission source sectors
    - Seltzer, K. M., Pennington, E., Rao, V., Murphy, B. N., Strum, M., Isaacs, K. K., & Pye, H. O. (2021). Reactive organic carbon emissions from volatile chemical products. *Atmospheric Chemistry and Physics*, *21*(6), 5079-5100.
  - Pesticide profile (eliminating “unknown” from profile)
  - Minor corrections to existing profiles
- Species Properties Table update
  - special thanks to H. Pye and the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) team
  - Updated the entire species properties table to assign a “representative” species for those species that are lumps of species. Ensures a consistent approach to estimating the chemical and physical properties when exact values are not known.

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; should be easier to find compounds
  - Can also use CAS or the DSSTX number (used by Computational Toxicology)
  - Users can visualize/compare profiles

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Questions?

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