IMPROVING EPA'S SPECIATE PROGRAM

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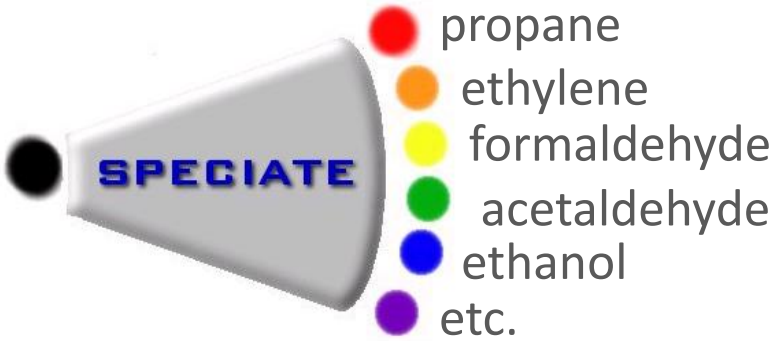
OVERVIEW

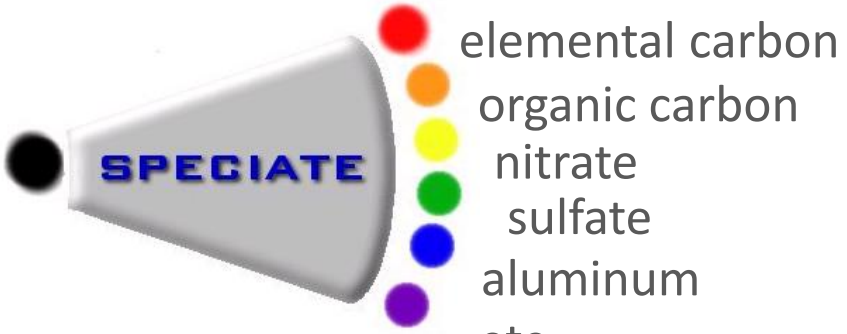
- What is SPECIATE?
- Uses of SPECIATE
- SPECIATE 5.1 Highlights
  - New Profiles
  - Structure changes
- Updated Speciation Tool Release
- Profiles used in modeling and priorities for New/Updated Data
- Guidelines for Data Developers
- Next Steps

SPECIATE

- Database containing the speciation profiles from specific emissions source types for volatile organic compounds (VOCs), particulate matter (PM) emission and other pollutants. Includes fields specifying:
  - Emission source category (e.g., wildfires, oil and gas production)
  - Weight percent of PM/VOC chemical species
  - Test methods, year, reference(s), etc.



VOC



$PM_{2.5}$

Mercury

PURPOSE OF SPECIATE DATABASE

- To identify, organize and make available relevant total organic gas and PM speciation profile data
  - Data can be from EPA, state agencies, peer-reviewed literature, and other relevant data sources
- To provide metadata elements for the users of speciation data
  - This includes the results of a quality review performed by the Work group
  - Description of the study, test methods, references
  - Data to support the volatility basis set (VBS) species for the modeling of organic aerosols in a chemical transport model

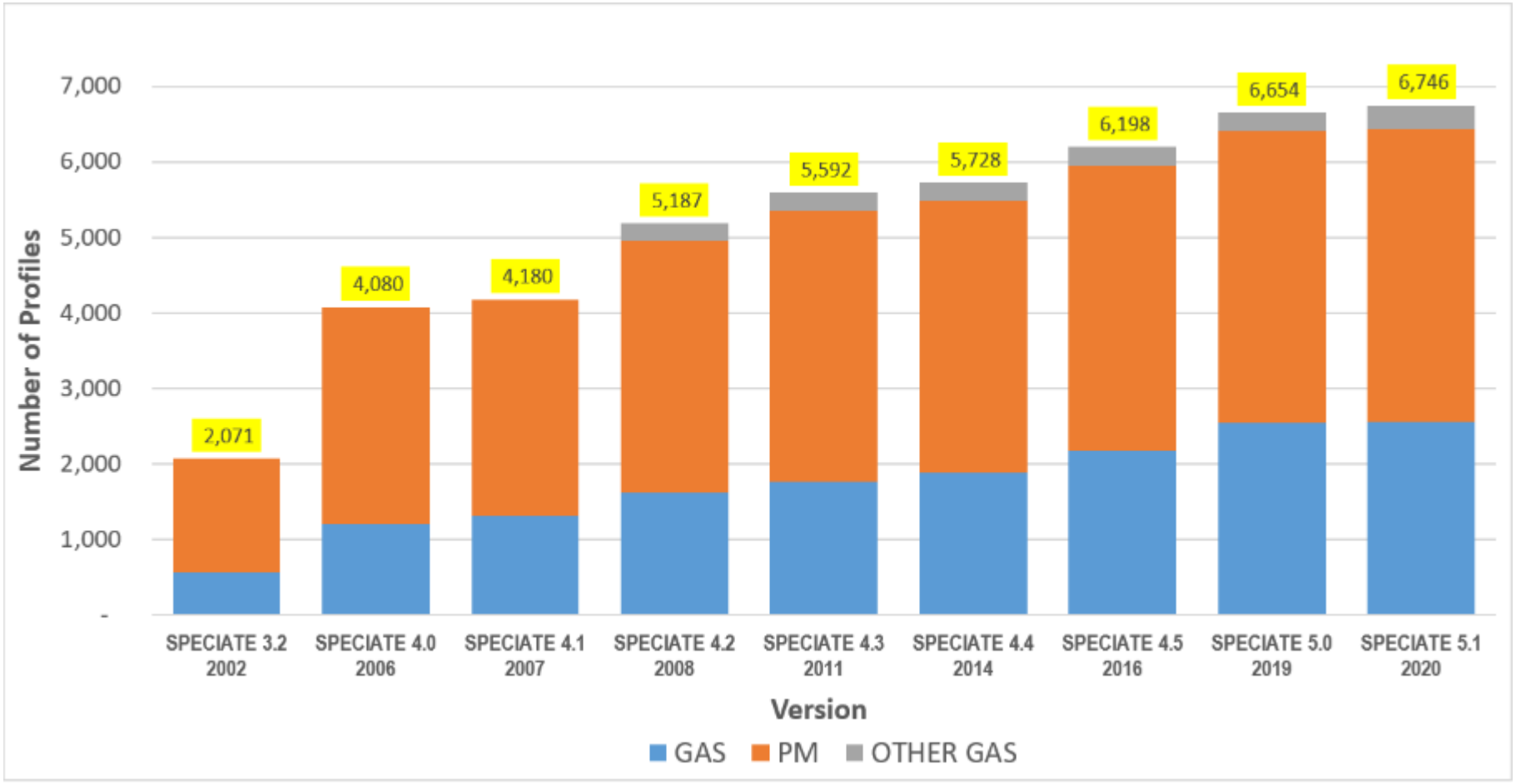
PRIORITY USE OF SPECIATE – AIR QUALITY MODELING

- Regulatory model applications
  - Air quality standards
  - Sector and transport rules
- Research model development
  - Secondary organic aerosol treatment
  - Chemical mechanisms
  - Specific sector analysis: Volatile Chemical Products, Oil and Gas, Biomass burning
- 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
  - Annual reporting for the Convention on Long-Range Transboundary Air Pollutant (LRTAP)
  - 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)
  - Arctic deposition study
  - EPA's Black Carbon Report to Congress
- National Emissions Inventory (NEI) PM species
- Estimate air toxics emissions (NEI, other inventories)
- Source apportionment

SPECIATE 5.1: EXPANSION OF THE DATABASE



SPECIATE 5.1
6,746 profiles

# of Profiles Added:
16 Gas,
18 PM2.5
58 mercury

Each version is a cumulative update of the previous version.

GAS PROFILES ADDED FOR SPECIATE 5.1

- Oil and Gas
  - Gas composition data for 3 counties in Pennsylvania (3 profiles)
  - Williston and Central Montana Uplift gas composition (some flash gas) (5 profiles)
  - Uinta basin raw gas from gas and oil wells, and flash gas from oil tanks and condensate tanks (6 profiles) – provided using the Data Developer's guide
- Marine vessel – composite of MOVES with Emission Factors derived from Commercial Marine Vessel Tanker study (1 profile)
- Diesel headspace composite - composite of existing profiles generated for version (1 profile)

PM PROFILES ADDED FOR SPECIATE 5.1

- Biomass burning
  - Forest and grass fire from lab and some field testing conducted by EPA in North Carolina, Oregon, Kansas, Minnesota, Montana (16 profiles)
  - Sugar cane burning PM2.5 profile (1 profile)
- Mobile
  - Corrected diesel bus exhaust – profile based on Environment Canada data (1 profile)

MERCURY PROFILES ADDED FOR SPECIATE 5.1

- Explained in "Development of Mercury Speciation Factors for EPAs Air Emissions Modeling Programs"
- Electric generation coal and petcoke profiles (composited from existing profiles) resulting from test data gathered from the 1999 Information Collection Request in support of the Clean Air Mercury Rule (44)
- Profiles from or derived from 2008 Global Atmospheric Mercury Assessment, Arctic Monitoring Assessment Programme (AMAP) – e.g., fuel combustion, incineration, cremation, metal production, non-combustion industrial average (7)
- Mobile profiles (composited from existing profiles) from EPA testing (2)
- Geothermal energy production – from 1977 paper (1)
- Portland cement kiln exhaust profile from industry-provided data (c. 2016) (1)
- Chlor-Alkali profile derived from 2003 paper (1)
- Elemental profile for a few sources – e.g., fluorescent lamps, dental amalgam (1)
- Particulate profile for Portland Cement clinker cooler (1)

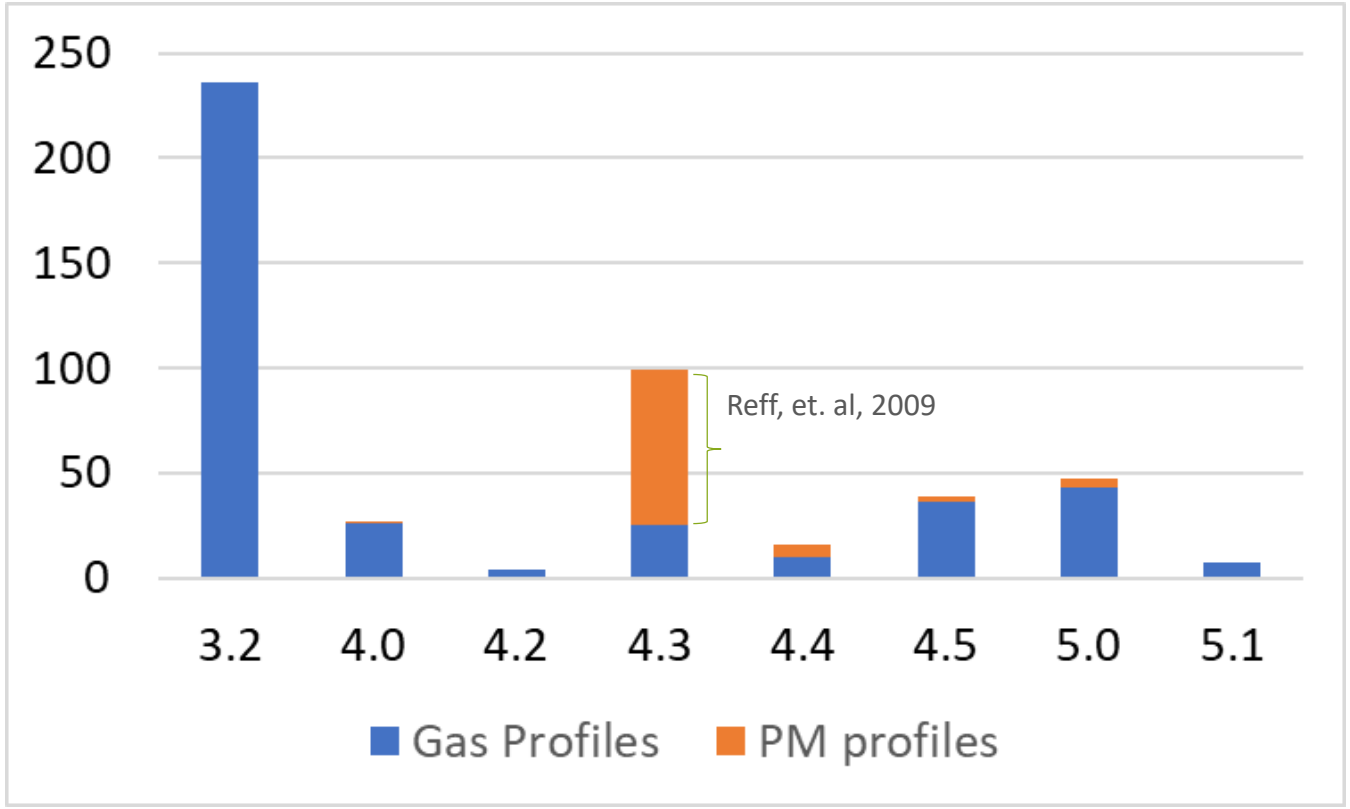
OTHER IMPROVEMENTS

- Data base structure and metadata
  - Reference structure – use of Reference Code
  - Updated CAS numbers and added synonyms for SPECIATE species
  - Added a field to support more automated mass reconstruction calculations
  - Populated all category level 1, 2 and 3 fields
  - Revised Quality Score (QSCORE) ratings and added QSCORE descriptive value
    - 22-30 = excellent (155 profiles)
    - 16-21 = good (358 profiles)
    - 8-15 = fair (17 profiles)
    - <7 = poor (0 profiles)
- Qlik SPECIATE data Browser – lets you find profiles, species and visualize profile weight percents

RELEASED SPECIATION TOOL 5.0 AND SMOKE REPORT ENHANCEMENTS

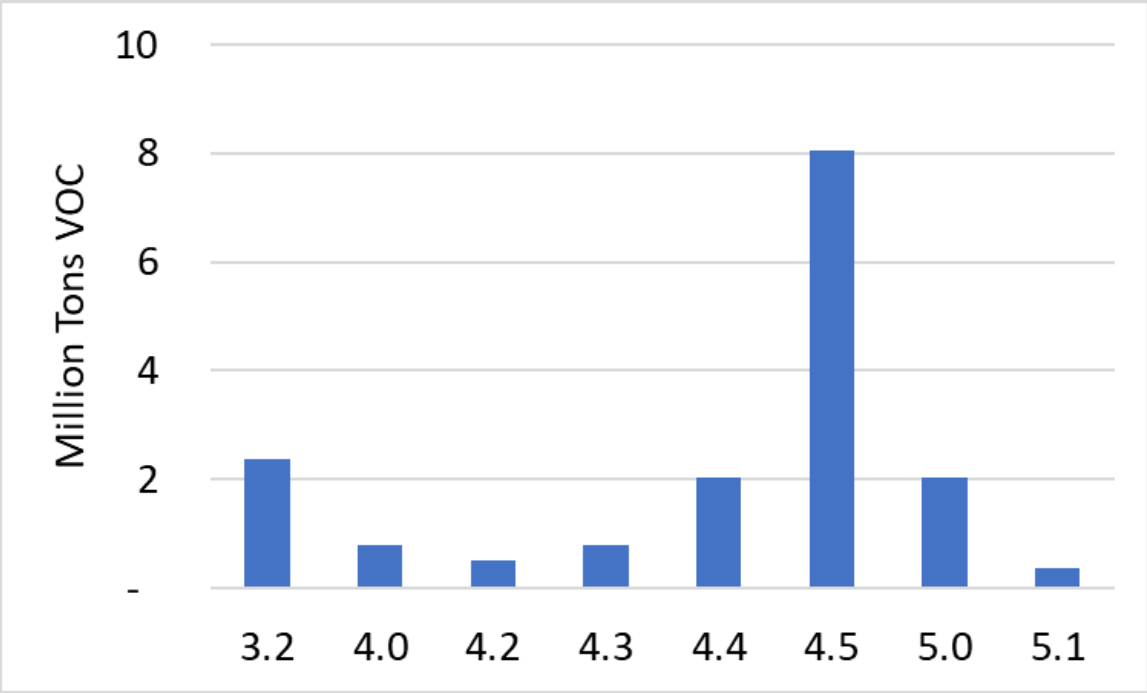
- Speciation Tool allows user to convert SPECIATE profiles to model-ready profiles (GSPRO) for SMOKE
- Speciation Tool 5.0 uses SPECIATE 5.0 (you can add any 5.1 profiles)
  - Mechanism mapping to mechanism-specific model species, IVOCs
  - Supports speciation profiles to integrate inventory hazardous air pollutants (HAPS) with VOCs
  - Create PM-AE6 profiles
  - Supports multiple gas phase mechanisms – CB6, CRI, SAPRC07T, RACM2
- Enhanced speciation summaries produced by SMOKE - Can get speciation summaries by SCC, pollutant and profile even when assigning multiple profiles to a source (i.e., 50% profile 1, 50% profile 2)

PROFILES USED IN MODELING (2017) BY SPECIATE VERSION

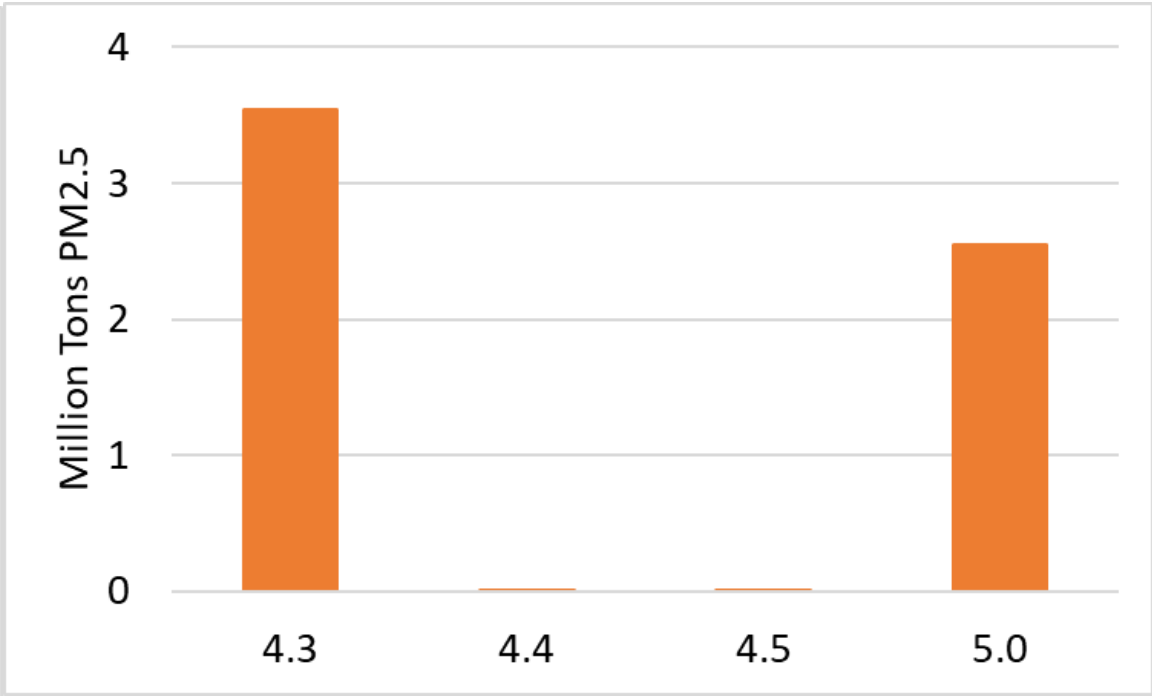


- Thousands of NEI source categories are mapped to a few hundred profiles
  - 475 profiles used in the platform (387 VOC; 88 PM)
  - Most are still from older versions of SPECIATE; (SPECIATE 3.2 released in 2002)

PROFILES USED BY MASS



SPECIATE 4.5 mass dominated by fires
(biogenic VOC is excluded in the above)



SPECIATE 4.3 mass dominated by dust (unadjusted for meteorology)
SPECIATE 5.0 by correction to fires (still old study; just recomposited)
Onroad excluded from PM analysis

SYSTEMATIC APPROACH: PRIORITY NEEDS

- **An assessment of important SPECIATE profiles in the EPA emissions modeling platform and current data gaps**
  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
  - Consumer Products (more broadly, volatile chemical products which also includes coatings and graphic arts)
- Appropriate source matching between literature and NEI

SPECIATION PROFILE NEEDS – HAP/VOC CONSISTENCY PERSPECTIVE (1)

- SPECIATE profile weight percentages generally do not match HAP inventory estimates, which may be more up to date or based on source-specific testing, material balance or emission factors
- HAPs in the NEI are used for VOC speciation for sources for which HAPs can be integrated with VOC; naphthalene, benzene, formaldehyde, acetaldehyde and methanol (NBAFM) that are explicit in CB6
- Focus on point sources and nonpoint sources for which we cannot integrate the inventory HAPs with the inventory VOC to create consistency between speciated emissions with NEI emissions
- Method: Identify profiles associated with non-integrated sources where speciated NBAFM is most different from inventory NBAFM
- Nonpoint
  - 0122 Bar Screen Waste Incinerator
  - 2489 Composite of 15 Fugitive Emission Profiles from Petroleum Storage Facilities - 1993
  - CARB3103 CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE) (naphthalene)
  - 0121 Open Burning Dump - Landscape/Pruning

SPECIATION PROFILE NEEDS – HAP/CAP INTEGRATION PERSPECTIVE (2)

- Point sources- profiles where inventory NBAFM is most different from Speciated NBAFM (non-integrated sources)
  - 2489 Composite of 15 Fugitive Emission Profiles from Petroleum Storage Facilities - 1993
  - 2485 Composite of 21 Fugitive Emission Profiles from Petroleum Industry Facilities - 1993
  - 2462 Composite of 3 Fugitive Emission Profiles from Chemical Mfg. Facilities (7% benzene)
  - 1084 Residential Wood Combustion (C-1 - C-6)
  - 0003 External Combustion Boiler - Natural Gas
  - 1001 Internal Combustion Engine - Natural Gas
  - 0332 Printing Press - Lithography Inking and Drying
  - 0007 Natural Gas Turbine

DATA FOR PROFILES FROM MANY SOURCES

- Quarterly literature search
  - No papers reflecting speciation of U.S. sources
- EPA ORD Test Programs
- State Agencies
- Western Region Air Partnership (WRAP)
- Desert Research Institute
- Reaching out to researchers at technical conferences

GUIDELINES FOR DATA DEVELOPERS

- Created documentation to help guide researchers/data developers create data (voluntarily) and publications that will be useful to SPECIATE
  - Created a ‘How-To’ document
  - Created a template for data developers to use when voluntarily developing profiles
  - Created an email for questions/comments/collaboration requests: **SPECIATE_WG@EPA.GOV**

WHAT IS NEXT?

- Currently working on an update to the database: SPECIATE 5.2
  - New profiles – hydronic heater study, updated consumer products profiles
  - Improved data from volatility and reactivity perspectives
    - Adding/updating Gas and PM profiles with disaggregation of *unspeciated* organic mass into volatility classes (e.g. IVOCs, SVOCs, LVOCs)
    - Populating new metadata fields with particle loading and temperature to enable reconciliation with inventory bulk PM and VOC emission factors.
    - Add metadata to reflect species reactivity to form ozone (e.g., MIR)
- Plan to complete Standard Operating Procedures document by December 2020

USEFUL LINKS

- Database: https://www.epa.gov/air-emissions-modeling/speciate-2
- Documentation: https://www.epa.gov/air-emissions-modeling/speciate-4
- Browser: https://www.epa.gov/air-emissions-modeling/speciate-0
- Guidelines for Data Developers: https://www.epa.gov/air-emissions-modeling/speciate-3
- Emission Modeling Tools (SMOKE and Speciation Tool): https://www.cmascenter.org/
- SPECIATE Email box SPECIATE_WG@epa.gov

SPECIATE Data Browser 5.1

Filter Menu

Profile - Detail | Profile - Basic | Profile List | Species Properties | Weight % (bar) | Weight % (pie) | Revisions

Profile Data - Detail

All profiles | All species

PROFILE COD...	PROFILE_NAME	PROFI...	PROFILE_...	CATEGORY_LE...	CATEGORY_LEVEL_2_Sector_Equipment	CATEGORY_LEVEL_3_Fuel_Product	MASTE...	VER!
1	Natural Gas - Untreated - Gas Well	95257	GAS	Volatilization	Oil And Gas; Well	Produced Gas	TOG	4.5
1	Natural Gas - Untreated - Gas Well	95257	GAS	Volatilization	Oil And Gas; Well	Produced Gas	TOG	4.5
1	Natural Gas - Untreated - Gas Well	95257	GAS	Volatilization	Oil And Gas; Well	Produced Gas	TOG	4.5
1	Natural Gas - Untreated - Gas Well	95257	GAS	Volatilization	Oil And Gas; Well	Produced Gas	TOG	4.5
1	Natural Gas - Untreated - Gas Well	95257	GAS	Volatilization	Oil And Gas; Well	Produced Gas	TOG	4.5
1	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	PRBCB_R	GAS	Volatilization	Oil And Gas; Well	Produced Gas; Coal Bed Methane	TOG	4.5
1	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	PRBCB_R	GAS	Volatilization	Oil And Gas; Well	Produced Gas; Coal Bed Methane	TOG	4.5
1	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	PRBCB_R	GAS	Volatilization	Oil And Gas; Well	Produced Gas; Coal Bed Methane	TOG	4.5
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6,746								