Improvements to EPA's SPECIATE Database: SPECIATE5.0

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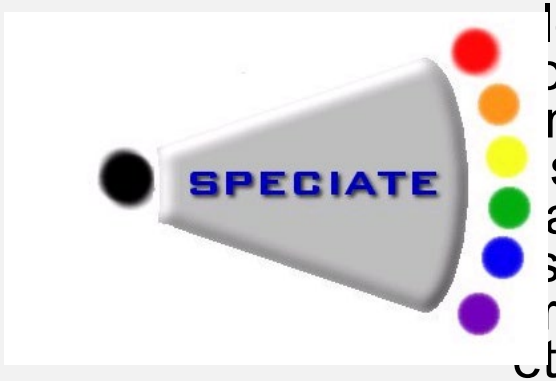
What Is SPECIATE

Repository of source-based speciation profiles that provide the chemical composition of organic gas such as volatile organic compounds (VOC), and particulate matter (PM)

VOC

ropane
ethylene
formaldehyde
acetaldehyde
ethanol
tc.

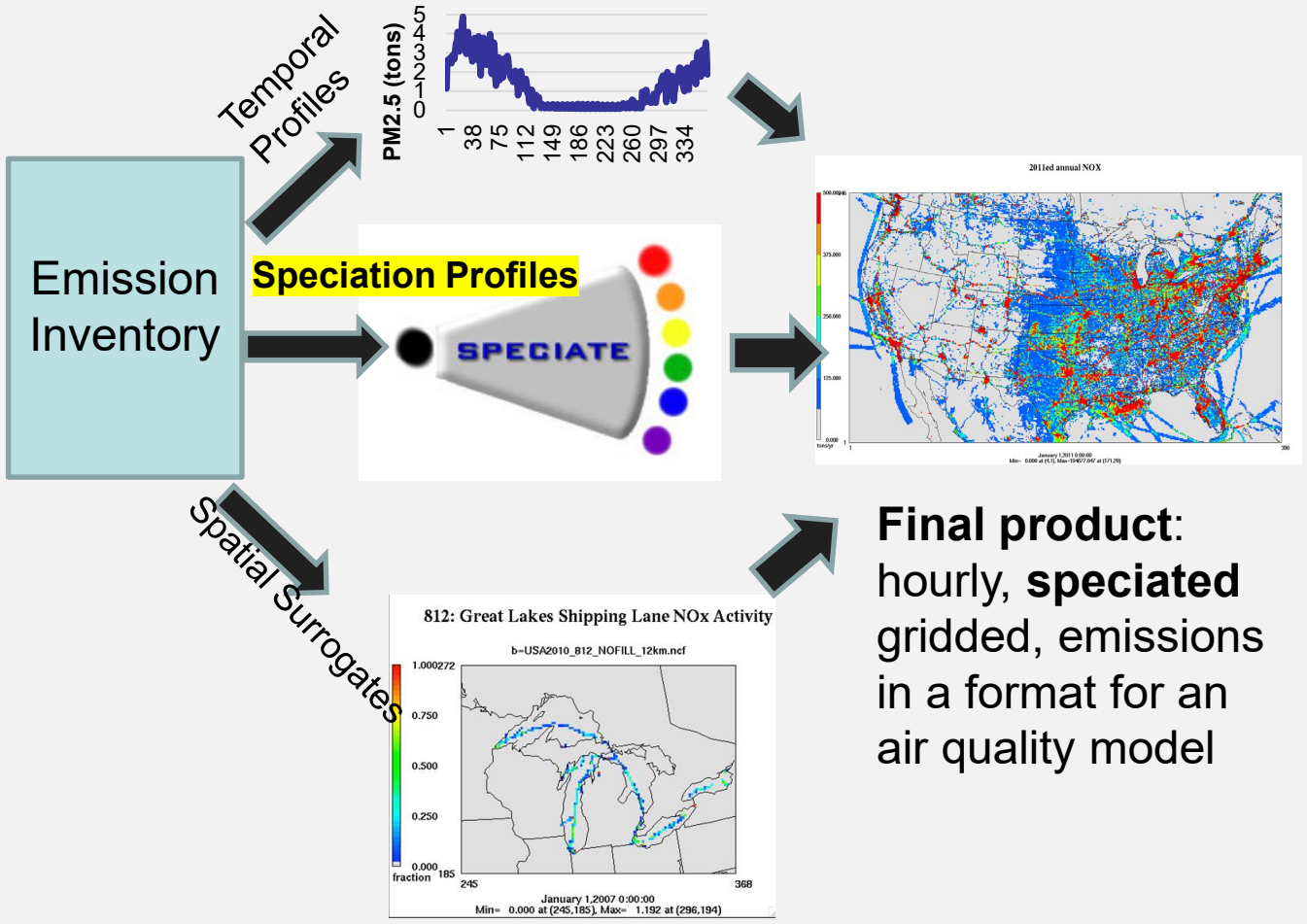
$PM_{2.5}$



lemental carbon
organic carbon
nitrate
sulfate
aluminum
silicon
ron
tc.

SPECIATE As Part of Emissions Preparation for Photochemical Air Quality Modeling

SMOKE software system performs temporal allocation, speciation and spatial allocation



Final product: hourly, **speciated** gridded, emissions in a format for an air quality model

- VOC and $PM_{2.5}$ need to be speciated into chemical components for photochemical modeling
- Each speciation profile is cross-referenced to an inventory source by source classification code (SCC), pollutant, and potentially by region
- Thousands of SCCs in the NEI are mapped to a few hundred profiles

Other Key Uses

- Estimate black carbon and organic carbon for use in carbon emission assessments and inventories
  - Black Carbon Report to Congress
  - Arctic deposition study
- Source apportionment
- Estimate air toxics emissions

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SPECIATE

Types of Profiles in SPECIATE

- GAS – Organic gas, based on VOC or total organic gases (TOG)
- GAS-VBS – Used for volatility basis set (VBS) treatment in air quality models (contains intermediate volatility explicit and lumped species based on saturation vapor pressure)
- PM-Simplified – Model-ready for AE5 aerosol mechanism
- PM-AE6 – Model-ready for AE6/AE7 aerosol mechanism
- PM-VBS – Model-ready for VBS treatment in chemical transport models (contains organic carbon and non-carbon organic matter lumped species broken out by saturation vapor pressure; includes SVOCs)
- PM – Any other PM (i.e., not model-ready)
- OTHER – Mercury, NOX, semi-volatile VOC (SVOC)

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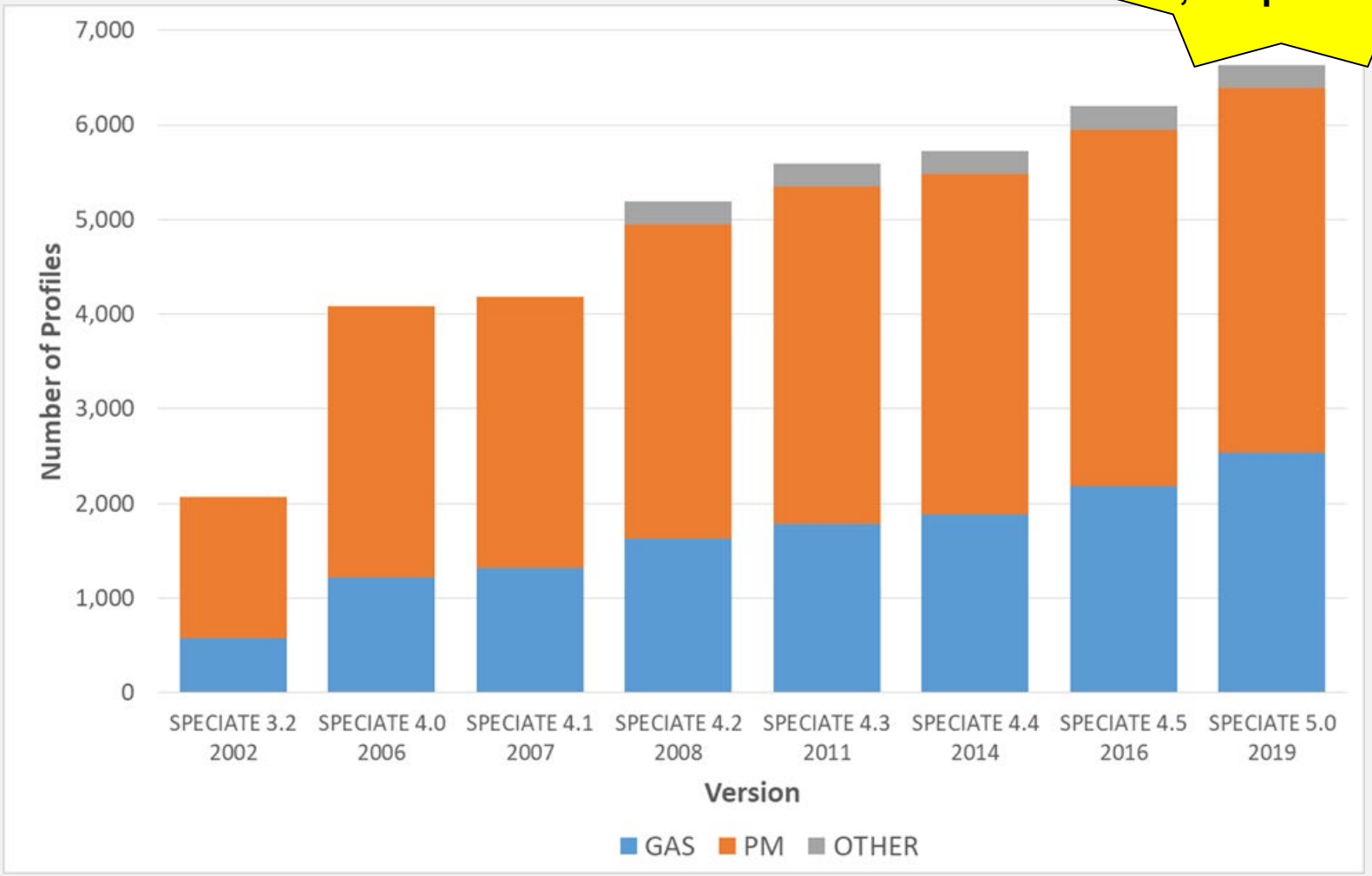
Expansion of the SPECIATE Database

SPECIATE5.0: 6,654 profiles



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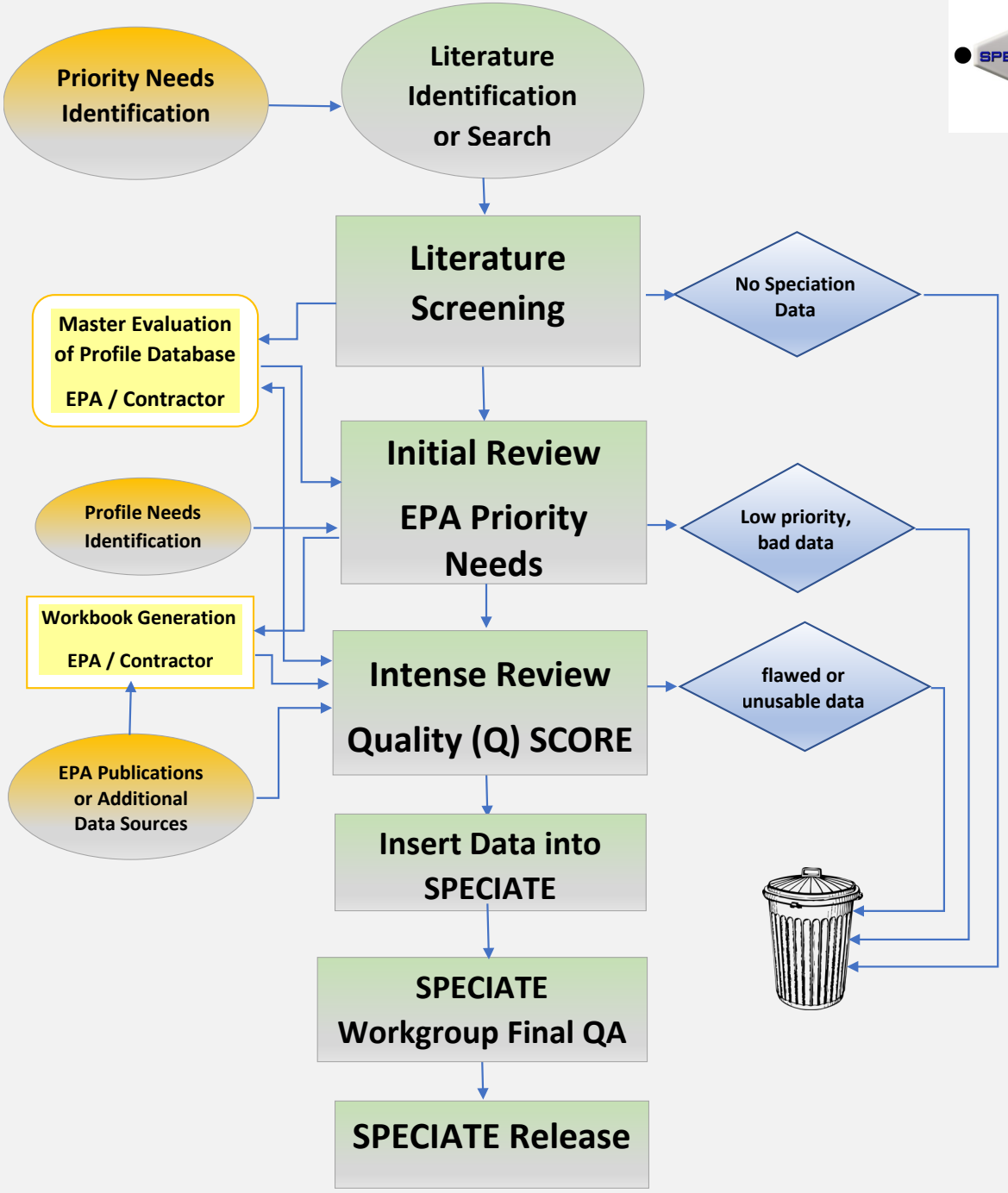
How Profiles are Added



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Updates to SPECIATE 5.0

- Database design (improved Microsoft Access® structure)
- Additional metadata fields
- Corrected nonVOC fields (SPECIES_PROPERTIES)
  - Siloxanes fixed - resulting from EPA research on organic aerosol formation from volatile chemical products
- Added profiles
- Improved online browser
- Overall improvements to the SPECIATE program
  - Needs Analysis (Bray, et al., Atmospheric Environment, June 2019)
  - Guidelines for data developers

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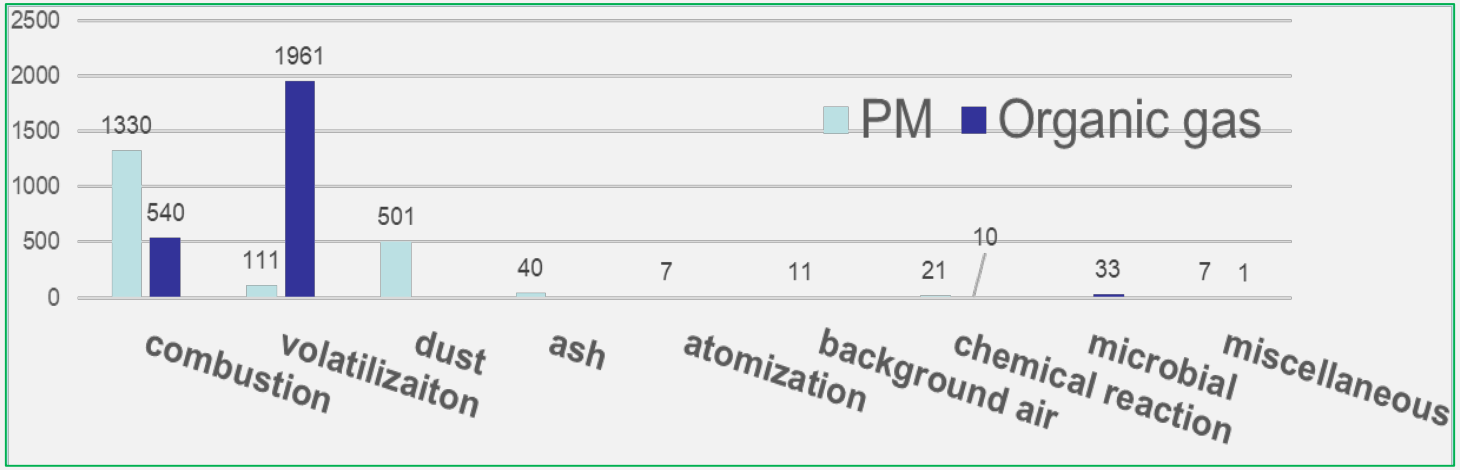
SPECIATE

Profile Categorization Fields

- CATEGORY_LEVEL_1_Generation Mechanism
  - 9 distinct values, most are “combustion” or “volatilization”



- CATEGORY_LEVEL_2_Sector_Equipment
  - ~ 200 distinct values, e.g., “biomass burning; prescribed fire” or “biomass burning; fireplace”
- CATEGORY_LEVEL_3_Fuel_Product
  - ~500 distinct values, e.g., “wheat straw” or “rice straw” or “juniper”

Other Metadata Fields Added

- QSCORE
- Master_Pollutant emission rate
- Species emission rates
- Mass Overage Percent
- Organic loading
- Particulate loading
- Species vapor pressure
- Species oxygen to carbon ratio

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Additional Quality Review Process "QSCORE"

- Evaluation criteria focused on
  - Reference
  - Relevance of data (emission source reflects current technology)
  - Quality test program
  - Documentation on sampling/analytical method
  - Profile Completeness
  - Data reduction/statistics
- Our Cross-Office SPECIATE Workgroup develops the QSCORE for every profile via team discussions

Improved Documentation

- Now providing Excel® workbooks showing calculations from the raw data (e.g., journal article) to SPECIATE profiles
- Improved access to references
  - Digital Object Identifiers (DOIs) for literature references
  - Web links to reports where available on internet
  - Documents that are not readily available via web link are posted on our ftp site

New Profiles – SPECIATE 5.0

- Added Profiles
  - 375 new GAS profiles for a total of 2,550
  - 80 new PM profiles for a total of 3,854 (PM, PM-AE6, PM-SIMPLIFIED)
  - 6 PM-VBS and 4 GAS-VBS profiles

- Considering at least the following SPECIATE5.0 profiles for our air quality modeling platform:

Gas (TOG):
- Sugar cane burning
- Consumer products (multiple)
- Corrected heavy duty diesel
- Wyoming oil and gas (multiple)
- Livestock (multiple)

PM (PM2.5):
- Marine Vessel AE6
- Corrected wildfire/prescribed fire
- Natural gas combustion
- Aircraft

New SPECIATE Browser

- Provides database access for the non-Access® user
- Ability to search, view and download profiles and/or metadata, species, and export them into Excel®
- Filter by any metadata field; sort any field
- Construct your own table with fields of interest
- *LINK:* https://www.epa.gov/air-emissions-modeling/speciate
- *Tip: don't use internet explorer – google chrome is fine*

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Browser – Profile Info view gives you ALL fields

Profile Info

Search on any field

ROW COUNT	PROFILE CODE COUNT	CATEG...	CATEGORY_LEVEL_2_Sector_Equipment	CATEGORY_LEVEL_3_ Fuel_Product	PROFILE_NAME	MASTER
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at -10 oC, 4-stroke, oxidation catalyst	PM
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at 20 oC, 4-stroke, oxidation catalyst	PM
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at -10 oC, 2-stroke	PM
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at 20 oC, 2-stroke	PM
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at -10 oC, 2-stroke, oxidation catalyst	PM
1	1	Combustion	Mobile; Onroad	Diesel	Diesel Exhaust - Bus at 20 oC, 2-stroke, oxidation catalyst	PM
1	1	Combustion	Biomass burning; Prescribed fire	Southeast conifer	Composite Profile - Prescribed fire southeast conifer forest	TOG
1	1	Combustion	Biomass burning; Prescribed fire	Southwest conifer	Composite Profile - Prescribed fire	TOG
330,083	**6,654**					

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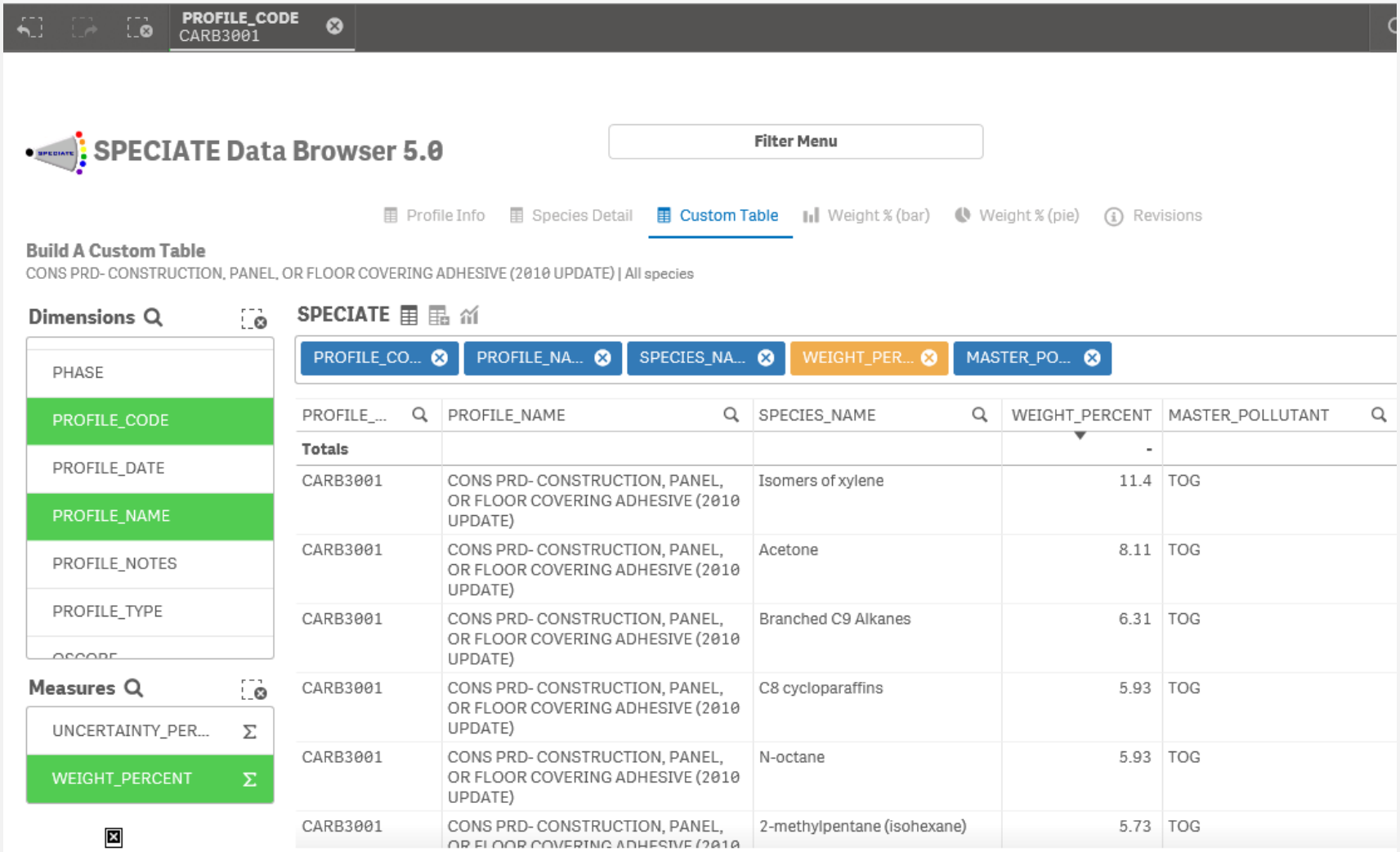
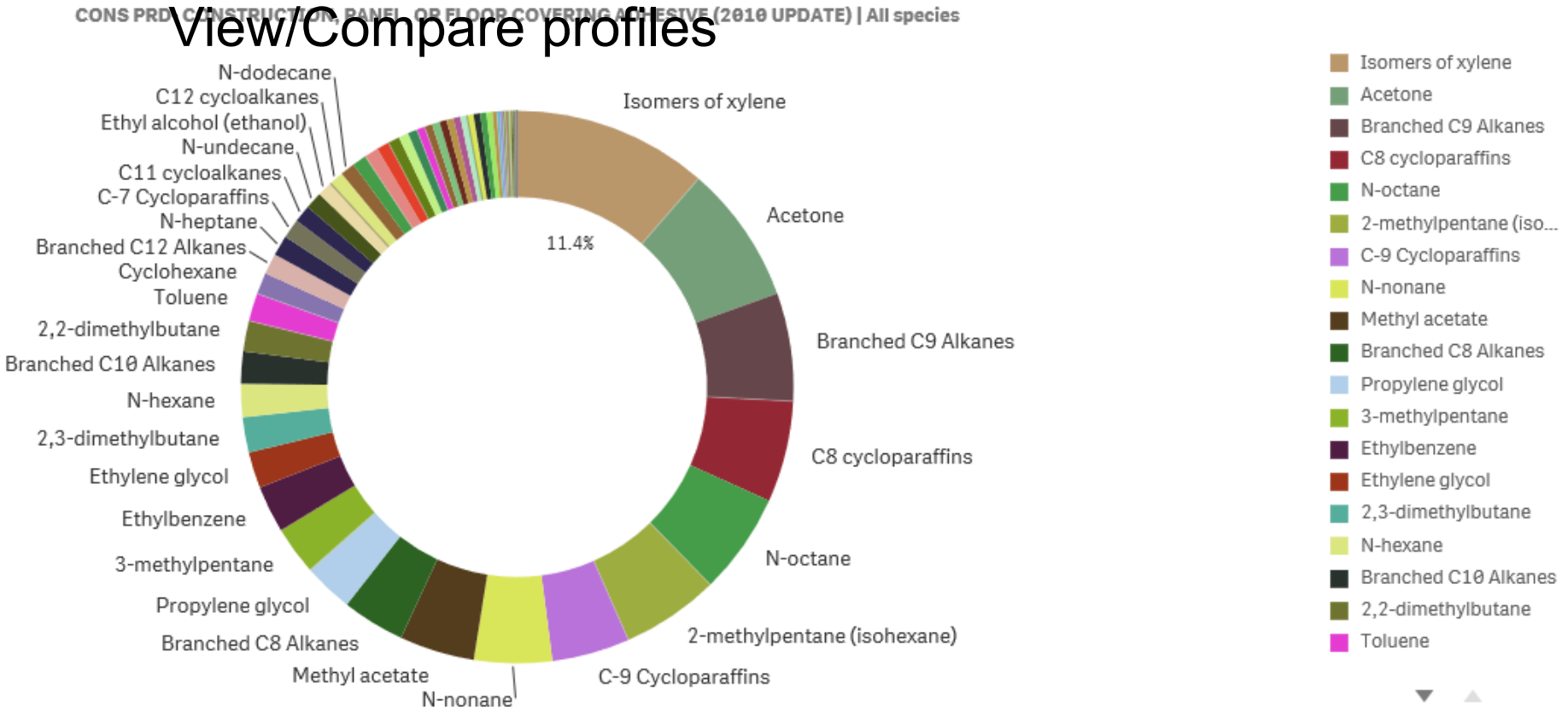
Browser – Custom Table

Selected one profile



Browser – View a Profile

View/Compare profiles



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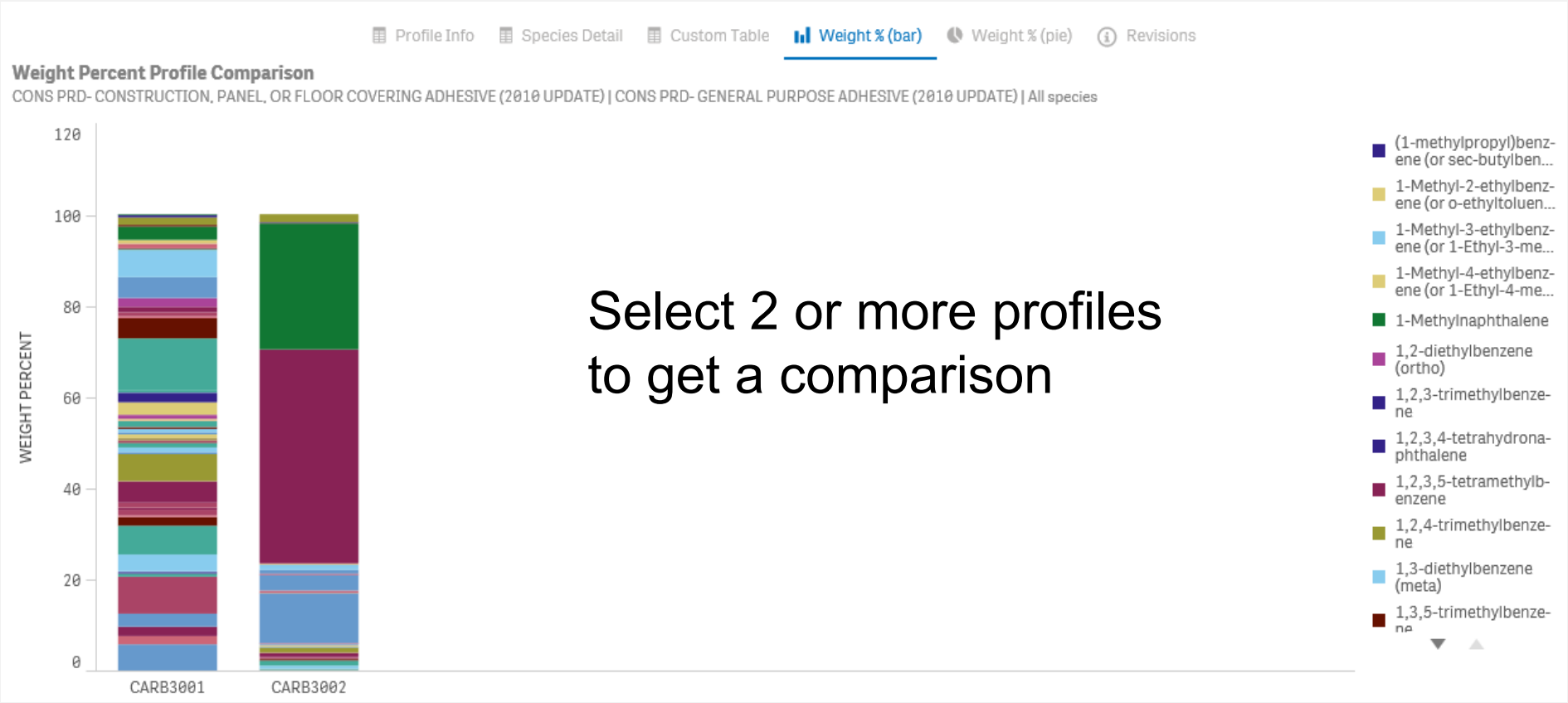
Browser – Compare 2 Profiles



Guidelines for Data Developers

- Discusses completeness, quality and documentation
- Data should fully characterize the source emissions (an entire suite of species)
- For PM emission source profiles, the size fraction of the PM should always be included
- Template with examples and further explanation of metadata fields provided as part of the guidelines document
- Data may be voluntarily emailed to SPECIATE_WG@epa.gov

Future Work

- Provide updates to SPECIATE more frequently
- Additional outreach to researchers on our data needs
- Continue to improve the database

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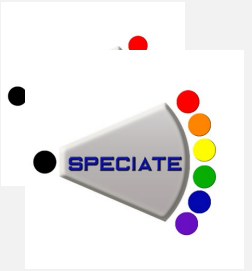

The End

For more information

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