

Assessment of important SPECIATE profiles in EPA's emissions modeling platform and current data gaps

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What is SPECIATE?

- Database containing the speciation profiles from specific source types for both volatile organic compounds (VOCs) as well as particulate matter (PM) emissions
- Allows total VOC and PM_{2.5} to be speciated into chemical components for photochemical modeling
- Each speciation profile is cross-referenced to an emissions inventory source by Source Classification Code (SCC), by pollutant, and potentially by region
- Used for policy, planning and research purposes

Objective

Needs assessment to determine what the highest priority is for new and/or improved emission profiles for photochemical modeling applications.

Project Goals

- 1. To determine which profiles are most prominent in the EPA 2014 modeling platform based on VOC emitted mass, VOC reactivity, and PM₂₅ emitted mass
- 2. To prioritize a running list of papers and reports that have been identified, but not yet added to SPECIATE
- 3. To identify gaps in the current literature in order to encourage research groups to measure speciation from sources that will be the most beneficial to the US EPA's modeling and policy efforts

Steps Taken

Step 1: Identify most used profiles \rightarrow Ranked profiles by total mass assigned in EPA's most recent 2014 modeling platform **Step 2:** Conduct in depth evaluation \rightarrow **Profile analysis criteria:** Top 90% of PM_{2.5} emissions (by mass) and top 65% of VOC emissions

(by mass) \rightarrow Further examinations: quality of profile, age, appropriateness, region

Step 3: Rank-order profiles by highest priority for updates to profiles or updates to SCC-mapping



Figure 1. NOAA Climate Regions [Source: https://www.ncdc.noaa.gov/monitoringreferences/maps/us-climate-regions.php]

Focusing on 3 regions for this presentation:

Southeast
Southwest
Northeast

U.S. Environmental Protection Agency

Most Prominent Profiles By Emissions Mass



Sub-Bituminous Combustion-Composite Wood Fired Boiler-Composite Nonroad Gasoline Exhaust-Composite Charbroiling - Composite Mineral Products-Avg-Composite

Petroleum Industry-Avg-Composite Other

Figure 2. Top ~93% PM_{2.5} profiles by emission mass on a national scale compared with top profiles on a regional scale for the Southeast, Northeast and Southwest US.



Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells Natural Gas Flare Profile with DRE >989

Oil and Gas Production - Composite Profile - Glycol Dehydrator, Uinta Basin

Oil and Gas Production - Untreated Natural Gas. Uinta Basir

Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - E10 ethanol gasoline

Gasoline Headspace Vapor - 10% Ethano

Degreasing: Cold Cleaning (Batch, Conveyor, Spray Gun)

- All Automotive Aftermarket Products
- Household Products
- Solvents And Coating Related Products
- Crude Oil Storage Tanks
- Mineral Products Asphaltic Concrete
- Composite Profile Wildfire northwest conifer forest
- Prescribed Fire SW conifer Fireplace wood combustion - pine wood

Figure 3. Top ~65% of VOC profiles by emission mass on a national scale compared with top profiles on a regional scale for the Southeast, Northeast and Southwest US.

Pesticides

Prioritization of Profiles - Methodology

Criteria	Points assigned	
Age	Old	1
	New	0
Reliability of Reference	Low	2
	Medium	1
	High	0
SCC issue?	No	0
(e.g. mismatch between sources tested and SCC assigned in modeling platform)	Major	1
	Minor	2
Maximum % weight among regions	> 12%	4
(emissions assigned to profile within region/total emissions in	8-12%	3
region)	4-8%	2
	< 4%	1
Known error in data?	No	0
	Yes	2
Study region applicable?	Yes	0
	Νο	1

Table 1. Priority ranking system for the criteria of interest. Profiles are ranked based on the criteria in order to assess priority of individual profiles.





Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells Oil and Gas -Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Well Oil and Gas Production - Composite Profile - Oil Tank Vent Gas, Uinta Basi Oil and Natural Gas Production - Condensate Tanks

Natural Gas Production

Gasoline Headspace Vapor - 0% Ethano

Architectural Coatings: Solvent Borne and water borne

Personal Care Product Pesticides/FIFRA-Regulated Products

Graphic Arts - Printing Wildfire boreal forest

Prescribed Fire NW conife

Prescibed Fire - SE Conit Open Burning Dump - Landscape/Pruning

Prioritization of Profiles – Preliminary Results

PM₂ Priority Ranking

Profile	Profile Name	Score	Ranking
91102	Wildfires – Composite	9	1
91103	Agricultural Burning – Composite	9	1
91106	HDDV Exhaust – Composite	7	2
91110	Sub-Bituminous Combustion – Combustion	7	3
91113	Nonroad Gasoline Exhaust – Composite	7	3
91109	Prescribed Burning – Composite	7	3
91101	Agricultural Soil – Composite	6	4
91112	Natural Gas Combustion – Composite	5	5
91108	Paved Road Dust – Composite	4	6
91100	Unpaved Road Dust – Composite	4	6
91105	Residential Wood Combustion – Composite	3	7
91116	Charbroiling – Composite	3	7

Table 2. Priority ranking for PM_{25} source profiles in need of updates. **VOC Priority Ranking**

Profile	Profile Name	Score	Ranking
0121	Open Burning Dump – Landscape/Pruning	6	1
4642	Fireplace Wood Combustion – Pine Wood	5	2
2487	Composite of 7 Emission Profiles from Crude Oil Storage Tanks – 1993	5	2
8949	Natural Gas Production	5	2
95421	Composite Profile – Prescribed Fire Southeast Conifer Forest	5	2
3145	Consumer Products Composite: Pesticides/FIFRA-Regulated Products	4	3
3146	Consumer Products Composite: Household Products	4	3
3147	Consumer Products Composite: Personal Care Products	4	3
95425	Composite Profile – Wildfire Boreal Forest	4	3
95422	Composite Profile- Prescribed Fire Southwest Conifer Forest	4	3
1191	Graphic Arts – Printing	3	4

Table 3. Priority ranking for VOC source profiles in need of updates.

Findings on High Priority Profiles

- and are not applied to the appropriate SCCs
- smoldering and flaming phases of fire
- west but is applied nationally
- inappropriate SCCs (i.e. trash burning)

Future Directions

Future Directions

- Add VOC reactivity analysis
- For each region, continue project:
- applied in the modeling framework]
- receive high priority for inclusion into SPECIATE
- the literature

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• Many profiles used for both PM_{2.5} and VOC are derived from fairly old measurements

• Wildfire and prescribed burning profiles currently do not distinguish between

• Profile 91102 (Wildfire – Composite) included measurements from fencepost burning • Profile 91103 (Agricultural Burning – Composite) only representative of crops in the

• Profile 0121 (Open Burning Dump –Landscape/Pruning) is applied to some

• Expand study regions to each NOAA Climate region and conduct analysis again

Step 4: Determine if there are existing SPECIATE profiles in other versions that may be better than what is currently being used, or if a composite of existing SPECIATE profiles may be better [There are currently profiles created in SPECIATE that are not being

Step 5: Browse the current literature, including the existing reference list, to identify existing profiles that could satisfy needs identified in step 3 and recommend that those

Step 6: Communicate with research community (journal article/presentations at conference, etc.) about high-priority sources for which no appropriate profiles exist in