

New Upgrades to EPA's SPECIATE Database

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What Is SPECIATE?

- ❖ Repository of Speciation Profiles for:
 - » Volatile Organic Compounds (VOC)/Total Organic Gases (TOG), and
 - » Particulate Matter (PM).

SPECIATE Users

- ❖ Air Quality Modelers (model species profiles);
- ❖ Receptor Modelers (source profiles – markers);
- ❖ Emission Inventory Preparers (TAP/HAP inventories, GHG inventories); and
- ❖ Planners - rule development (e.g. regulations of product formulation based on reactivity).

SPECIATE Update Project

- ❖ Incorporated new speciation data with 1,263 PM and 406 VOC source profiles;
- ❖ Revise the SCC – Profile cross reference file;
- ❖ Revise the TOG-to-VOC Conversion Factors Table; and
- ❖ Develop Average and Composite speciation profiles.

Additional Information for New SPECIATE Profiles

- ❖ Comprehensive TOG/VOC speciation (about 160 new compounds);
- ❖ Many new PM profiles speciated for particle-bound SVOC (e.g. gas/diesel exhaust PM, fireplaces, forest fires); and
- ❖ Meta Data – profile quality rating, vintage, sampling and analytical methods, number of samples collected, references, % of mass speciated, control device, region, other data.

New Profile Data Sources

- ❖ EPA;
- ❖ DOE National Renewable Energy Lab;
- ❖ State Agencies (CARB, TCEQ);
- ❖ Coordinating Research Council;
- ❖ Society of Automotive Engineers;
- ❖ Desert Research Institute; and
- ❖ Scientific Literature.

Important Source Sectors with New SPECIATION Data

1999 NEI VOC Sectors			1999 NEI PM ₁₀ Sectors		
Rank	(ton/day)	Primary Source	Rank	(ton/day)	Primary Sources
1	9906	Gasoline Motor Vehicle/Nonroad	1	1235	Prescribed/Wildfires
2	3275	Surface Coatings	2	995	Agricultural Equipment
3	3118	Gasoline Refueling	3	910	Unpaved Roads
4	2355	Degreasing	4	520	Electric Generation
5	2201	Diesel Vehicles	5	505	Diesel On-Highway
6	1733	Automotive Aftermarket	6	490	Quarry, Mining
7	1581	Heavy-Duty Gasoline Vehicles	7	374	Electric Generation Coal
8	1491	Pesticides	8	344	Woodstoves
9	1343	Misc. Solvents and Adhesives	9	250	Wood Boiler
10	1087	Asphalt	10	216	Light Duty Gasoline
11	906	Non-Industrial Adhesives	11	176	Paved Road Dust
12	903	Oil and Gas Production	12	161	EGU Oil
13	720	Wood Furniture	13	147	Pulp and Paper Sulfate
14	685	Personal Care Products	14	137	Agricultural Dust
15	679	Auto Refinishing	15	134	Nonroad Equipment
16	677	Fireplaces	16	101	Gray Iron Foundries
17	631	Dry Cleaning			
18	606	Graphic Arts			
19	540	Household Products			

Important New VOC Data

- ❖ Fireplaces and wood stoves: previous profile had only PAHs and aldehydes; new profile has 22% methane and many other TOG species;
- ❖ Forest fires/prescribed burning: were assigned to the RWC profile. New profiles include foliar fuel burning based on EPA data;

Important New VOC Data (cont.)

- ❖ Petroleum Storage: previous profile dominated by xylenes (22%) with little highly-volatile compounds and oxygenates. New profile data dominated by pentanes, MTBE, butanes, and other highly volatile species; xylenes <2%; and
- ❖ Consumer Products, Coatings and Related Products: previous profile had only one species – n-butyl alcohol. New composite profile based on CARB data includes over 100 species.

Important New VOC Data (cont.)

- ❖ Solvent Mixtures: e.g. mineral spirits, Stoddard solvent, petroleum distillates, naphtha, aliphatic hydrocarbons now available for use or to resolve these mixtures within existing profiles.

Impacts of the New VOC Data

(Portion of SPECIATE3.2 #1201 –
Diesel Engine VOC Exhaust, circa 1980)

Pollutant	Percent	Pollutant	Percent
C-2 Compounds	19.96	C-10 Compounds	3.52
Formaldehyde	8.61	C-16 Compounds	3.49
C-1 Compounds	5.8	C-13 Compounds	3.43
C-3 Compounds	5.21	C-17 Compounds	3.06
C-14 Compounds	4.45	Acetaldehyde	2.91
C-15 Compounds	4.35	C-22 Compounds	0.59
C-6 Compounds	4.3	Benzaldehyde	0.55
C-4 Compounds	4.08	C-25 Compounds	0.54
C-11 Compounds	3.58	C-23 Compounds	0.48

Impacts of the New VOC Data

(Portion of the New SPECIATE VOC Profile – Diesel Truck Exhaust)

Pollutant	Percent	Pollutant	Percent
Acetaldehyde	22.62	Acetylene	2.49
Formaldehyde	12.07	2-methyl-2-propenal	2.16
Propionaldehyde	7.58	Toluene	2.15
Crotonaldehyde	7.25	N-butane	2.07
Ethylene	4.63	Benzaldehyde	2.06
Methyl ethyl ketone	4.06	Acrolein	1.84
Acetophenone	2.76	Heptanal	1.73
		Octanal	1.68

Impacts of the New VOC Data (Comparison of Model Species - Diesel)

Model Species	Symbol	SPECIATE 3.2 Profile #1201		New Diesel Profile		Difference, % (Old-New) / Old	
		Split Factor	Mass Fraction	Split Factor	Mass Fraction	Split Factor	Mass Fraction
Paraffins	PAR	0.0224	0.4734	0.0159	0.2530	29	47
Olefins	OLE	0.0019	0.0381	0.0017	0.0607	11	-59
Toluene	TOL	0.0017	0.0438	0.0005	0.0371	71	15
Xylene	XYL	0.0002	0.0050	0.0003	0.0278	-50	-456
Formaldehyde	FORM	0.0029	0.0861	0.0045	0.1347	-55	-56
Aldehydes	ALD2	0.0014	0.0472	0.0091	0.3597	-550	-662
Ethylene	ETH	0.0035	0.0665	0.0017	0.0463	51	30
Non-reactive	NR	0.0142	0.2397	0.0044	0.0807	69	66

Important New PM Data

- ❖ Comprehensive PM speciation profiles: EC, OC, ions, elements, and particle-bound SVOCs (e.g. PAHs).

Impacts of the New PM Data

- ❖ Better characterization of toxic air pollutant emission estimates from particle-bound SVOC (e.g. PAHs);
- ❖ Better elemental and organic carbon emission estimates (e.g. diesel combustion).

Next Steps

- ❖ Develop Compositated Profiles
- ❖ Develop TOG-to-VOC conversion factors
- ❖ Prepare SCC-Profile cross reference table
- ❖ User interface

SPECIATE PROJECT WEB SITE

PROJECT WORK PLAN

PROGRESS REPORTS

MEETINGS

DOCUMENTS

CONTEXT DIAGRAM

ASSIGNMENTS/ACTIVITY

SPECIATE VERSIONS

DISCUSSION FORUM



What's New:

06 April 2005 - The [Context Diagram](#) has been updated.

06 April 2005 - Agenda for today's meeting is available on the [Meetings](#) page, and [here](#).

30 March 2005 - Website Debut. Material posted in Project Work Plan, Progress Reports, Meetings, Documents, Context Diagram, and Discussion Forum sections.

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