FINAL REPORT

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SPECIATE Version 4.5 Database Development Documentation

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Abstract

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of volatile organic gas and particulate matter (PM) speciation profiles of air pollution sources. Some of the many uses of these source profiles include: (1) creating speciated emissions inventories for regional haze, PM, greenhouse gas (GHG), and photochemical air quality modeling; (2) estimating hazardous and toxic air pollutant emissions from PM and organic gas primary emissions; (3) providing input to chemical mass balance (CMB) receptor models; and, (4) verifying profiles derived from ambient measurements by multivariate receptor models (e.g., factor analysis and positive matrix factorization).

This report documents the updates that EPA applied to SPECIATE version 4.4 to develop the SPECIATE 4.5 database. EPA generated SPECIATE 4.5 by appending 296 volatile organic gas profiles and 182 PM profiles to the SPECIATE 4.4 database. In total, the SPECIATE 4.5 database includes 6,206 PM, volatile organic compound (VOC), total organic gases (TOG), and Other Gases profiles. The SPECIATE 4.5 database also contains a table titled "Semi-volatile Organic Compounds (SVOC) Splitting Factors" that provides suggested SVOC partitioning factors between PM and gaseous phases.

Abt Associates, Inc. developed SPECIATE 4.5 through a collaboration involving EPA's Office of Research and Development (ORD) and Office of Air Quality Planning and Standards (OAQPS) in Research Triangle Park, NC, and Office of Transportation and Air Quality (OTAQ) in Ann Arbor, MI. This report first discusses the uses and structure of the SPECIATE 4.5 database in Chapters I and II, respectively. Chapter III identifies the major data sources and presents the methods used to develop the new profiles not previously included in SPECIATE. Chapter IV provides important notes and comments on the use of the profiles, Chapter V briefly discusses source profile preparation methods, and Chapter VI provides the references for this report.

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Acknowledgments

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- EPA National Exposure Research Laboratory (NERL)
- EPA National Risk Management Research Laboratory (NRMRL)
- EPA Office of Air Quality Planning and Standards (OAQPS)
- EPA Office of Transportation and Air Quality (OTAQ)

The authors would like to thank the members of EPA's SPECIATE Workgroup and those individuals that provided data for the SPECIATE 4.5 database. The primary contact for the project is Mr. Michael Kosusko, the EPA Work Assignment Manager (WAM) for this project; the Alternate WAM is Dr. Madeleine Strum. The Workgroup is coordinated by Mr. Kosusko, and staffed by air quality professionals from the EPA's Office of Research and Development and the Office of Air and Radiation. As of September 2016, the committee members include:

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Contents

Tables

Figures

Acronyms and Abbreviations

AAAR	American Association for Aerosol Research
ACE	Air, Climate and Energy Program
ACS	American Chemical Society
AMAD	Atmospheric Modeling and Analysis Division, EPA
APPCD	Air Pollution Prevention and Control Division, EPA
AQAD	Air Quality Assessment Division, EPA
ASD	Assessment and Standards Division, EPA
CARB	California Air Resources Board
CAS	Chemical Abstracts Service
CED	Community & Ecosystem Division
CMAQ	EPA Models-3 Community Multi-scale Air Quality Modeling System
CMB	chemical mass balance
CRC	Coordinating Research Council
DOE	Department of Energy
DRI	Desert Research Institute
EC	elemental carbon
ERMD	Emissions Research and Measurement Division (Environment Canada)
EPA	Environmental Protection Agency
EPHD	Environmental Public Health Division, EPA
ES&T	Environmental Science and Technology
FID	flame ionization detector
GC	gas chromatography
GHG	greenhouse gas
HDDV	heavy-duty diesel vehicle
HEASD	Human Exposure and Atmospheric Sciences Division, EPA
HEID	Health and Environmental Impacts Division, EPA
HPLC	high performance liquid chromatography
ID	identification
IO	immediate office
IOAA	Immediate Office of the Assistant Administrator, EPA
ITN	internal tracking number
kg	kilogram
km	kilometer
LDDV	light-duty diesel vehicle
mg	milligram
MO	metal-bound oxygen
MTBE	methyl t-butyl ether
MW	molecular weight
NAICS	North American Industry Classification System
NCEA	National Center for Environmental Assessment, EPA
NEI	National Emissions Inventory
NERL	National Exposure Research Laboratory, EPA
NHEERL	National Health and Environmental Effects Research Laboratory, EPA
NMHC	non-methane hydrocarbons

NMOG	non-methane organic gas
NPD	National Program Director
NPRI	National Pollutant Release Inventory (Environment Canada)
NREL	National Renewable Energy Laboratory
NRMRL	National Risk Management Research Laboratory, EPA
NVFEL	National Vehicle and Fuel Emissions Laboratory
OAQPS	Office of Air Quality Planning and Standards, EPA
OAR	Office of Air and Radiation, EPA
OC	organic carbon
OEP	Office of Ecosystem Protection, EPA Region 1
OM	organic matter
OPRA	Office of Partnerships and Regulatory Assistance
ORD	Office of Research and Development, EPA
OTAQ	Office of Transportation and Air Quality, EPA
PAHs	polycyclic aromatic hydrocarbons
PAMS	photochemical assessment monitoring station
PM	particulate matter
PM_{10}	particulate matter with an aerodynamic diameter ≤ 10 micrometers
$PM_{2.5}$	particulate matter with an aerodynamic diameter ≤ 2.5 micrometers
PNCOM	particulate non-carbon organic matter
RFG	reformulated gasoline
RPCS	Research Planning and Coordination Staff, EPA
RTP	Research Triangle Park
SAROAD	Storage and Retrieval of Aerometric Data
SIC	Standard Industrial Classification
SPPD	Sector Policies and Programs Division, EPA
SRS	Substance Registry System
SVOC	semi-volatile organic compounds
TAME	t-amylmethyl ether
TAP	toxic air pollutant
TC	total carbon
TCEQ	Texas Commission on Environmental Quality
THC	total hydrocarbon
TOG	total organic gases
TOR	thermal optical reflectance
TOT	thermal optical transmission
UV	ultraviolet-visible
VOC	volatile organic compounds
WAM	Work Assignment Manager

CHAPTER I. Introduction

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of volatile organic gas and particulate matter (PM) speciation profiles of air pollution sources (Simon et al., 2010). A speciation profile outlines the chemical composition of an emission source in weight percent of PM or volatile organic gas. Speciation data are developed through source testing by laboratories and research institutes, and are often published in journal articles. Each profile in SPECIATE is supplemented with metadata to document the source of data. There are instances where multiple profiles are available for the same source type. In these cases, the Workgroup develops composite profiles to better represent the emission source compositions (see Chapter IV, Section M for a description of composite profiles).

Some of the many uses of these emission profiles include: (1) creating speciated emissions inventories for regional haze, PM, greenhouse gas (GHG), and photochemical air quality modeling; (2) estimating hazardous and toxic air pollutant emissions from PM and organic gas primary emissions; (3) providing input to chemical mass balance (CMB) receptor models; and, (4) verifying profiles derived from ambient measurements by multivariate receptor models (e.g., factor analysis and positive matrix factorization).

The primary purpose of this project is to update the SPECIATE database to capture recent and scientifically-meritorious VOC, TOG, and PM speciation profile data available from EPA, state agencies, peer-reviewed literature and other relevant data sources. Recent SPECIATE databases (i.e., versions 4.0, 4.1, 4.2, 4.3, 4.4, and 4.5) allow for storage of important information underlying each profile (metadata such as sampling and analysis methods, normalization procedures, overall subjective profile quality ratings, etc.).

The SPECIATE Workgroup (Workgroup) consists of EPA and Abt Associates, Inc. staff, university researchers, receptor/photochemical/dispersion modelers, emission inventory developers, and government agency staff. Members of the Workgroup contribute and/or gather data, and provide recommendations as to which specific speciation profiles should be added to the database.

The SPECIATE 3.2 database, which was released in 2002, contained profiles that are the result of testing and/or studies conducted in the 1980s, and in some cases, the 1970s. EPA released an updated SPECIATE database version 4.0 in November 2006 to capture more recent VOC and PM speciation profiles developed by EPA staff and other researchers. Since the release of SPECIATE 4.0, there have been numerous new profiles added to the database, resulting in SPECIATE versions 4.1, 4.2, 4.3, 4.4, and 4.5. The purpose of this report is to document the updates that EPA applied to SPECIATE 4.4 (see hyperlink below) to generate the SPECIATE 4.5 database and to describe additional work that could be performed to further improve the database. Copies of the SPECIATE 4.5 database can be obtained from the EPA Project Manager, Mr. Michael Kosusko (kosusko.mike@epa.gov) or downloaded from the EPA website: https://www3.epa.gov/ttn/chief/software/speciate/index.html.

The following is an overview of the SPECIATE 4.x versions:

SPECIATE 4.0 (2006) included a total of 4,080 PM and organic gas profiles (2,009 new profiles and 2,071 profiles carried forward from SPECIATE 3.2). SPECIATE 4.0 also included 1,360 new PM profiles (of which 95 are simplified profiles and 47 are composite profiles) and 649 organic gas profiles (of which 11 are composite profiles). The SPECIATE 4.1 database, which was never officially published by EPA, included a total of 4,180 PM and organic gas profiles (with 4,080 carried forward from SPECIATE 4.0). The primary update to the SPECIATE 4.1 database was the addition of 100 VOC profiles obtained from Environment Canada's National Pollutant Release Inventory (NPRI) database.

SPECIATE 4.2 (2008) included an additional 408 VOC profiles and 462 PM profiles. EPA changed the structure of the SPECIATE 4.2 database by adding a new category called Other Gases. This category contains speciated mercury, nitrogen oxides, and semi-volatile organic compounds (SVOC) which do not fall into VOC or PM profile categories. There are 237 Other Gases profiles incorporated into SPECIATE 4.2. The SPECIATE 4.2 database and later versions also contain a new table titled "SVOC Splitting Factors", which provides suggested SVOC partitioning factors in PM and gaseous phases based on a Schauer et al. study (1999; see memorandum in Appendix D for more details). Note that the partitioning factor of each SVOC species is not universal, but dependent on sampling conditions (e.g., temperature and pressure).

SPECIATE 4.3 (2011) added an additional 151 volatile organic gas (including TOG and VOC) profiles, 244 PM profiles, and 10 speciated mercury profiles. The majority of the new speciation profiles incorporated came from EPA and peer reviewed literature. Emission source sectors include internal combustion engine exhaust from onroad vehicles and marine vessels, gasoline and its evaporative emissions, ethanol fuel production, the pulp and paper industry, and several other stationary sources. Additionally, numerous profiles were added to support PM speciation compatibility with the AERO6 aerosol module in the CMAQ photochemical model (versions 5.0 and later). This model requires emissions of particulate non-carbon organic material (PNCOM), particulate-bound water, ammonium, sodium, chloride and 8 trace metals as distinct model species using the approach in Reff et al. (2009).

SPECIATE 4.4 (2014) includes comprehensive speciation of TOG profiles from oil and gas fugitive emissions, gasoline vehicle exhaust, VOC emissions from the dairy industry (including silages, other feedstuffs, and animal waste), gasoline vapor from enclosed fuel tanks, PM profiles from the Kansas City Light-Duty Vehicle Emissions Study (EPA, 2008), outdoor wood boiler aerosol emissions, and commercial aircraft jet engine PM emission profiles. In total, there were an additional 104 volatile organic gas profiles and 32 PM profiles included in the SPECIATE 4.4 database.

The **SPECIATE 4.5** (2016) database focuses on the incorporation of individual and composite volatile organic gas and PM profiles from the oil and natural gas sector, motor vehicle exhaust, biomass combustion, waste incineration, and tire and break wear emissions.

As of September 2016, the initiative to update SPECIATE to version 4.5 has produced:

- Additional "model-ready"[1] PM profiles following the method described in Reff et al. (2009);
- VOC-to-TOG conversion factors for applicable gas profiles;
- Suggested partitioning factors for SVOC compounds in gas and PM phases; and
- The SPECIATE 4.5 database with the following total number of profiles and unique species:
    - 3,782 PM profiles;
    - 2,175 organic gas profiles;
    - 249 Other Gases profiles;

[1] Model-ready PM profiles refer to PM profiles that are compatible with the requirements for CMAQ versions 5.0 and later

- 2,602 unique species; and
- Composite profiles for 85 (51 PM and 34 organic gas) source categories.

SPECIATE is expected to be an ongoing project that supports Agency research, regulation development and enforcement. The Workgroup has identified and prioritized numerous datasets for which profiles will be developed and added to future versions of SPECIATE. Comments and questions based on review of the database and documentation are welcome and may be directed to Mr. Michael Kosusko (kosusko.mike@epa.gov) or Dr. Madeleine Strum (Strum.Madeleine@epa.gov).

The remainder of this report discusses the structure and use of the SPECIATE 4.5 database in Chapter II, and then details the development of the profiles and supporting tables in Chapter III. Comments on the use of the profiles appear in Chapter IV and Chapter V briefly discusses source profile preparation methods. Chapter VI provides the references for this report. Tables A-1 and A-2 of Appendix A provide a summary of the organic gas and PM profiles in the SPECIATE 4.5 database, respectively. Appendix B provides a protocol for preparing profiles for the future versions of the SPECIATE database. Appendix C provides speciation profiles for unresolved mixtures of compounds listed as a single species. Appendix D provides SVOC partitioning factors and the methodology applied to prepare mobile source exhaust profiles in the SPECIATE database.

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CHAPTER II. SPECIATE Database

This chapter describes the organization of the SPECIATE 4.5 database. This includes subsections on the use of the database, the data dictionary, overall subjective profile quality rating criteria, and profile identification (ID) numbers.

A. Use of the Database

The SPECIATE 4.5 database is a data repository housed in a Microsoft Access® database file. In order to use the SPECIATE 4.5 database, Microsoft Access® 2002 or above must be installed. The current SPECIATE database and other relevant documentation can be downloaded from EPA's Clearinghouse for Inventories & Emissions Factors website (https://www.epa.gov/air-emissions-modeling/speciate-version-44-through-32). To facilitate inspection of the data by persons without detailed database manipulation skills, the queries VIEW_PM_PROFILES and VIEW_GAS_PROFILES have been added and are available on the Queries tab in MS Access. The VIEW_GAS_PROFILES query links the GAS_PROFILE, GAS_SPECIE, and SPECIE_PROPERTIES tables together to allow the user to view all of the fields in these tables when the query is run. The VIEW_PM_PROFILES query links the PM_PROFILE, PM_SPECIE, and SPECIE_PROPERTIES tables together to allow the user to view all of the fields in these tables when the query is run.

B. Database Design

The SPECIATE 4.5 database design appears in Figure 1. The design is based on suggestions from the October 2002 meeting of the SPECIATE Expert Panel held at the American Association for Aerosol Research conference in Charlotte, NC, as well as additional recommendations provided by EPA over the years.

PM profiles may be expressed over any PM size range (i.e., PM particle size ranges are not pre-determined). This capability is provided through the upper- and lower- size limit fields in the PM_PROFILE table. In instances in which multiple profiles (arising from multiple size distributions) result from a single study, the particle size range will be explicitly designated in the table. The SPECIATE 4.5 database can therefore accommodate species size distributions for any range. Future studies that require more particle size resolution can be accommodated, consistent with the expectations of future research.

Profiles for particulates, organic gases, and Other Gases continue to be housed in separate tables due to their slight variance in database architecture. Other tables, such as SPECIE_PROPERTIES and KEYWORD, are common to organic gases, particulates, and other gases.

The data dictionary (see Table 1 and subsection C below) is intended to be general and not specific to any particular database architecture. Accordingly, variance from the data dictionary expressions for some fields (e.g., Logical versus Boolean) may occur. Fields such as T_METHOD (sampling method) and ANLYMETHOD (analytical method) contain character expressions representing the respective method employed.

The profile tables include rating fields for profile vintage (V-rating), data sample size (D-rating), and expert judgment (J-rating). The Overall Objective Profile Quality Rating is the product of the V-rating and D-rating [see Chapter II.D (Profile Rating Criteria) for rationale regarding profile overall ratings].

The use of P_NUMBER as the primary key for the profiles tables has been retained from the previous versions of SPECIATE. This is the unique logical key when accessing common tables.

A REGION field is intended to house information on the geographic testing locale of certain profiles. For example, the VOC profiles based on Environment Canada's NPRI database can be identified by two-letter province abbreviations under the Region column in the Gas Profile table (e.g., BC stands for British Columbia) or gas profile numbers 7100 - 7199. NORM_BASIS indicates the aggregation of species by which the profile has been normalized [e.g., TOG, VOC, and PM with an aerodynamic diameter equal to or less than 10 micrometers (PM_{10})]. For the case where both a PM and GAS profile have been taken from the same study, the SIBLING field is used to identify the associated profiles.

The fields UNCERTAINT, UNC_METHOD, and ANLYMETHOD (see Table 1 and subsection C below) in the species table store species-specific uncertainty values, uncertainty methods, and analytical methods, respectively.

Figure 1. SPECIATE 4.5 Data Diagram

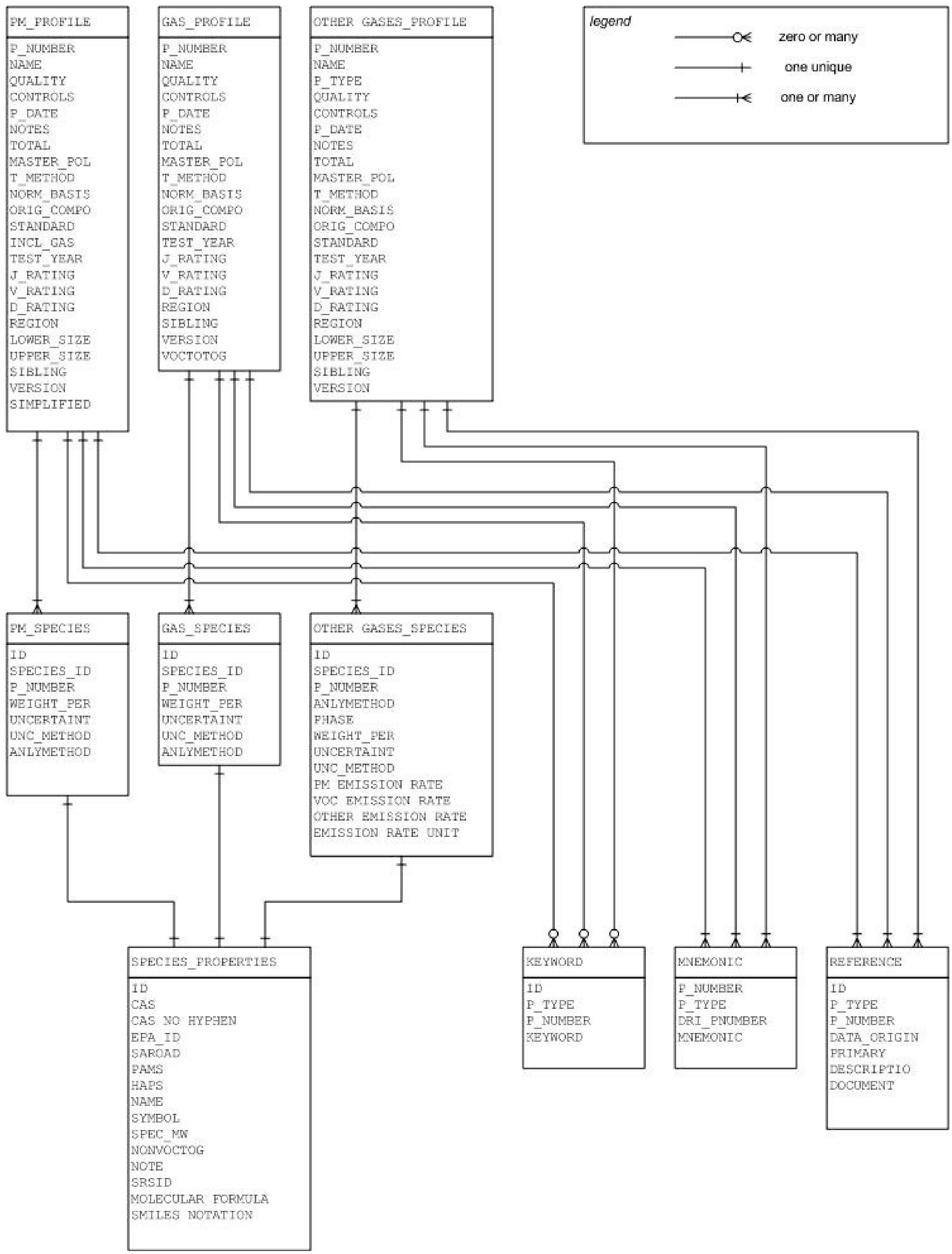

Table 1. Descriptive Data Dictionary

	Field	Type[1]	Length[2]	Decimals	Description
					PM_PROFILE Table
Primary key	P_NUMBER	C	10		PM Profile Number
	NAME	C	255		PM Profile Name
	QUALITY	C	3		Overall Objective Profile Quality Rating (A-E) of the profile (related to the products of the V and D ratings, see Chapter II.D for an explanation)
	CONTROLS	C	100		Emission Controls Description
	P_DATE	D			Date profile added (MM/DD/YYYY)
	NOTES	M			Notes
	TOTAL	N	6	2	Sum of species percentages for a given profile, excluding organic species, inorganic gases, and elemental sulfur in individual PM profiles (see Chapter IV.G "Avoiding Double Counting Compounds" of this report for rationale).
	MASTER_POL	C	5		Indicates the pollutant to be used in calculation. Allowed value: 'PM'. In the future, other values may be allowed (e.g., PM_PRI, PM_FIL, PM_CON)
	T_METHOD	M			Description of sampling method
	NORM_BASIS	C	25		Description of how profile was normalized (see Chapter IV.F for details)
	ORIG_COMPO	C	1		Specifies whether the profile is original or composite. Allowed values: 'C','O'
	STANDARD	L	1		Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
	INCL_GAS	L	1		Indicates whether or not the profile includes inorganic gas species (e.g., sulfur dioxide, hydrogen sulfide, oxides of nitrogen, etc.)
	TEST_YEAR	N	4	0	Indicates year testing was conducted
	J_RATING	N	4	2	Subjective expert judgment rating based on general merit (see Chapter II.D for an explanation)
	V_RATING	N	4	2	Vintage based on TEST_YEAR field (see Chapter II.D for an explanation)
	D_RATING	N	4	2	Data sample size rating based on number of observations (see Chapter II.D for an explanation)
	REGION	C	50		geographic region of applicability
	LOWER_SIZE	N	5	2	Identifies lower end of aerodynamic diameter particle size, micrometers
	UPPER_SIZE	N	5	2	Identifies upper end of aerodynamic diameter particle size, micrometers

Table 1 (continued)

	Field	Type[1]	Length[2]	Decimals	Description
Foreign key	SIBLING	C	10		GAS Profile number; samples taken from the same source and study, if available.
	VERSION	C	10		SPECIATE database version that a profile was added to
	SIMPLIFIED	L	1		Is the profile a PM Simplified Profile?
				PM_SPECIE Table	
Primary key	ID	N	9	0	Unique Identifier
Foreign key	SPECIE_ID	N	9	0	Species Identifier (The same as ID in SPECIE_PROPERTIES)
Foreign key	P_NUMBER	C	10		PM Profile number (Link to PM_Profile Table)
	WEIGHT_PER	N	7	3	Weight percent of pollutant (%)
	UNCERTAINT	N	7	3	Uncertainty percent of pollutant (%)
	UNC_METHOD	C	25		Description of method used to calculate uncertainty
	ANLYMETHOD	C	50		Description of analytical method (e.g., X-ray fluorescence spectroscopy, ion chromatography, etc.)
				REFERENCE Table	
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P (PM), G (Gas), Other gases (Other Gases)
Foreign key	P_NUMBER	C	10		Profile number (Link to PM_PROFILE and GAS_PROFILE tables)
	DATA_ORIGN	C	50		Source of data (e.g., EPA Air Pollution Prevention and Control Division (APPCD), Schauer, CARB, DRI, NPRI, Literature)
	PRIMARY	L			Designates a reference as primary. When a profile is based on multiple references, this field allows one reference to be tagged as the primary reference.
	DESCRIPTIO	M			Stores the descriptive information about the profile.
	DOCUMENT	M			Complete reference citation.
				GAS_PROFILE Table	
Primary key	P_NUMBER	C	10		GAS Profile Number
	NAME	C	255		GAS Profile Name
	QUALITY	C	3		Overall Objective Profile Quality Rating (A-E) of the profile (related to the products of the V and D ratings, see Chapter II.D for an explanation)
	CONTROLS	C	100		Emission Controls Description
	P_DATE	D			Date profile added (MM/DD/YYYY)
	NOTES	M			Notes

Table 1 (continued)

	Field	Type[1]	Length[2]	Decimals	Description
	TOTAL	N	6	2	Sum of organic gas species percentages for a given profile
	MASTER_POL	C	4		Indicates the pollutant to be used in calculation. Allowed values: 'VOC', 'TOG'. When methane is not measured in a study, ethane, acetone and other non-VOCs are removed from the profile and it is defined as a VOC profile.
	T_METHOD	M			Description of sampling method
	NORM_BASIS	C	25		Description of how profile was normalized
	ORIG_COMPO	C	1		Specifies whether the profile is original or composite. Allowed values: 'O','C'
	STANDARD	L	1		Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
	TEST_YEAR	N	4		Indicates year testing was conducted
	J_RATING	N	4	2	Subjective expert judgment rating based on general merit (see Chapter II.D for an explanation)
	V_RATING	N	4	2	Vintage based on TEST_YEAR field (see Chapter II.D for an explanation)
	D_RATING	N	4	2	Data sample size rating based on number of observations (see Chapter II.D for an explanation)
	REGION	C	50		Geographic region of source
Foreign key	SIBLING	C	10		PM Profile number; samples taken from the same source and study, if available.
	VERSION	C	10		SPECIATE database version to which profile was added
	VOCtoTOG	N	7	3	VOC to TOG conversion factor
				GAS_SPECIE Table	
Primary key	ID	N	9	0	Unique Identifier
Foreign key	SPECIE_ID	N	9	0	Species Identifier (Must be the same as ID in SPECIE_PROPERTIES)
Foreign key	P_NUMBER	C	10		GAS Profile Number (Link to GAS_PROFILE table)
	WEIGHT_PER	N	6	2	Weight percent of pollutant (%)
	UNCERTAINT	N	7	3	Uncertainty percent of pollutant (%)
	UNC_METHOD	C	25		Description of method used to calculate uncertainty
	ANLYMETHOD	C	50		Description of analytical method (e.g., gas chromatography (GC)/flame ionization detector (FID), GC/mass spectrometer (MS), high performance liquid chromatography (HPLC)/ultraviolet-visible (UV))

Table 1 (continued)

	Field	Type[1]	Length[2]	Decimals	Description
					OTHER GASES_PROFILE Table
Primary key	P_NUMBER	C	10		Other Gases Profile Number
	NAME	C	255		Other Gases Profile Name
	P_TYPE	C	25		Indicates Hg, SVOC, or NO/NO_2/HONO
	QUALITY	C	3		Overall Objective Profile Quality Rating (A-E) of the profile (related to the products of the V and D ratings, see Chapter II.D for an explanation)
	CONTROLS	C	100		Emission Controls Description
	P_DATE	D			Date profile added (MM/DD/YYYY)
	NOTES	M			Notes
	TOTAL	N	6	2	Sum of species percentages for a given profile
	MASTER_POL	C	5		Indicates the pollutant to be used in the calculation.
	T_METHOD	M			Description of sampling method
	NORM_BASIS	C	25		Description of how profile was normalized (see Chapter IV.F for details)
	ORIG_COMPO	C	1		Specifies whether the profile is original or composite. Allowed values: 'C','O'
	STANDARD	L	1		Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
	TEST_YEAR	N	4	0	Indicates year testing was conducted
	J_RATING	N	4	2	Subjective expert judgment rating based on general merit (see Chapter II.D for an explanation)
	V_RATING	N	4	2	Vintage based on TEST_YEAR field (see Chapter II.D for an explanation)
	D_RATING	N	4	2	Data sample size rating based on number of observations (see Chapter II.D for an explanation)
	REGION	C	50		Geographic region of applicability
	LOWER_SIZE	N	5	2	Identifies lower end of aerodynamic diameter particle size, micrometers
	UPPER_SIZE	N	5	2	Identifies upper end of aerodynamic diameter particle size, micrometers
Foreign key	SIBLING	C	10		Profile number; samples taken from the same source and study, if available.
	VERSION	C	10		SPECIATE database version to which profile was added
					OTHER GASES_SPECIE Table
Primary key	ID	N	9	0	Unique Identifier
Foreign key	SPECIE_ID	N	9	0	Species Identifier (The same as ID in SPECIE_PROPERTIES)

Table 1 (continued)

	Field	Type[1]	Length[2]	Decimals	Description
Foreign key	P_NUMBER	C	10		Other Gases Profile number (Link to OTHER GASES_Profile Table)
	ANLYMETHOD	C	50		Description of analytical method (e.g., GC/MS)
	PHASE	C	50		Indicates emissions were measured for PM, gaseous, or both phases.
	WEIGHT_PER	N	7	3	Weight percent of pollutant (%)
	SPECIES EMISSION RATE	N	7	3	Species emission rate
	UNCERTAINT	N	7	3	Uncertainty percent of pollutant (%)
	UNC_METHOD	C	25		Description of method used to calculate uncertainty
	PM EMISSION RATE	N	7	3	PM emission rate
	VOC EMISSION RATE	N	7	3	VOC emission rate
	OTHER EMISSION RATE	N	7	3	Other normalization basis (emission rate) other than PM or VOC, e.g., NO_x, total Hg. Indicate pollutant, e.g., 5.3 (NO_x), 3.6 (total Hg)
	EMISSION RATE UNIT	C	25		Units, e.g., mg/mile, mg/cycle
				KEYWORD Table	
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P, G
Foreign key	P_NUMBER	C	10		Profile Number (Link to PM_PROFILE and GAS_PROFILE Tables)
	KEYWORD	C	255		Keyword describing profile
				SPECIE_PROPERTIES Table	
Primary key	ID	N	9	0	Unique Identifier (Link to PM_SPECIES and GAS_SPECIES tables)
	CAS	C	50		Chemical Abstracts Service (CAS) number assigned to pollutant (with hyphens) (blank if no CAS)
	EPA_ID	C	50		EPA Chemical Identifier; provided by EPA Substance Registry System (SRS) for species without CAS numbers
	SAROAD	C	5		Storage and Retrieval of Aerometric Data (SAROAD) code
	PAMS	L	1		Is PAMS pollutant? (Yes or No)
	HAPS	L	1		Is Hazardous Air Pollutant? (Yes or No)
	NAME	C	255		Pollutant name
	SYMBOL	C	9		Standard chemical abbreviation (provided by Eric Fujita, DRI)
	SPEC_MW	N	6	2	Species molecular weight
	NonVOCTOG	L	1		Is this species regarded as a volatile organic gas?
	NOTE	C	250		Record notes

Table 1 (continued)

	Field	Type[1]	Length[2]	Decimals	Description
	SRS ID	C	50		EPA Substance Registry System Chemical Identifier
	Molecular Formula	C	50		Molecular formula
	Smiles Notation	C	100		Smiles notation
				MNEMONIC Table	
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P (PM), G (Gas)
Foreign key	P_NUMBER	C	10		Profile number (Link to PM_PROFILE and GAS_PROFILE tables)
	DRI_PNUMBR	C	6		DRI profile number (Original DRI profile numbers)
	MNEMONIC	C	60		Alphanumeric code unique to each profile. Used in CMB input files.

[1] Field types. C: Character; D: Date; L: Logical; M: Memorandum; N: Numeric.
[2] Length – number of characters allowed.

C. Data Dictionary

The SPECIATE 4.5 database is a Microsoft Access® relational database containing ten tables as described in Table 1 and Figure 1.

- The PM_PROFILE table includes, but is not limited to, profile number, name, notes on the profile, and descriptive information about the profile such as sum of species, test method, and normalization basis. Also incorporated in this table are the ratings including expert judgment, vintage, data sample size, and overall objective profile quality rating. The use of the ratings is detailed in Chapter II.D of this report.

- PM_SPECIE table includes the species identification number, the profile number associated with the species, the percentage of the species in the profile, the uncertainty associated with the percentage value, the method used to determine uncertainty, and a description of the analysis method used to determine the species percentage in the profile.

- The REFERENCE table includes information that characterizes the reference documents associated with the profiles, including whether or not a particular reference is the primary reference (thus allowing multiple and unlimited references for any profile).

- The GAS_PROFILE table includes, but is not limited to, profile number, name, notes on the profile, and descriptive information about the profile such as sum of species, test method, and normalization basis. Also incorporated in this table are the ratings including expert judgment, vintage, data sample size, and overall objective profile quality rating. The use of the ratings is detailed in Chapter II.D of this report. The GAS_PROFILE table contains Total Organic Gases (TOG), Non-Methane Organic Gases (NMOG), Volatile Organic Compounds (VOC), and Non-Methane Hydrocarbons (NMHC) profiles, depending on the available species and analytical methods. TOGs are compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate. VOCs contain similar compounds as TOGs, except VOCs exclude compounds that have negligible photochemical reactivity (i.e., exempt compounds). The EPA definition of VOC and a list of exempt organic gases are available at http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8

  Below are the relationships of TOG, VOC, NMOG, THC, and NMHC:

  TOG = VOC + exempt compounds (e.g., methane, ethane, various chlorinated fluorocarbons, acetone, perchloroethylene, volatile methyl siloxanes, etc.)

  TOG means "compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate." TOG includes all organic gas compounds emitted to the atmosphere, including the low reactivity, or "exempt VOC" compounds (e.g., methane, ethane, various chlorinated fluorocarbons, acetone, perchloroethylene, volatile methyl siloxanes, etc.). TOG also includes low volatility or "low vapor pressure" (LVP) organic compounds (e.g., some petroleum distillate mixtures). TOG includes all organic compounds that can become airborne (through evaporation, sublimation, as aerosols, etc.), excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate.

VOC means any compound of carbon that participates in atmospheric photochemical reactions. VOC excludes the mass of methane, ethane, acetone, carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate.

TOG = NMOG + methane

THC = NMHC + methane [contain only hydrocarbons (i.e., not oxygenated compounds like aldehydes) due to gas chromatography-flame ionization detector (GC-FID) measurement technique]

THC means organic compounds, as measured by a GC-FID. Notably, a FID does not accurately measure all of the mass of oxygenated organic gas, which influences the abundances of specific chemical compounds relative to the total in the measured organic compounds.

NMOG = NMHC + oxygenated compounds

- The GAS_SPECIE table includes the species identification number, the profile number associated with the species, the percentage of the species in the profile, the uncertainty associated with the percentage value, the method used to determine uncertainty, and a description of the analysis method used to determine the species percentage in the profile.

- The Other Gases_PROFILE table includes, but is not limited to, profile number, name, notes on the profile, and descriptive information about the profile such as sum of species, test method, and normalization basis. Also incorporated in this table are the ratings including expert judgment, vintage, data quality, and overall subjective profile quality rating. The use of the ratings is detailed in Chapter II.D of this report. The Other Gases Profiles are those that do not fit in the organic gas categories (TOG or VOC). Examples of the Other Gases Profiles are nitrogen oxides (NO, NO_2, HONO) and speciated mercury (elemental and oxidized mercury).

- The Other Gases_SPECIE table includes the species identification number, the profile number associated with the species, the percentage or emission rate of the species in the profile, the uncertainty associated with the percentage value, the method used to determine uncertainty, and a description of the analysis method used to determine the species percentage or emission rate in the profile.

- The KEYWORD table includes descriptive keywords of profiles. This information can be used in keyword-based searches for profiles.

- The SPECIE_PROPERTIES table includes the identifying numbers associated with the compounds that are species in the database, as well as other characteristic information such as molecular weight.

- The MNEMONIC table includes abbreviated profile names used in CMB receptor models.

D. Profile Rating Criteria

SPECIATE is a legacy application that the EPA and other environmental stakeholders have used for many years. The new profiles added to SPECIATE 4.0 and later versions were developed based on datasets that have become available since the release of SPECIATE 3.2, as described in Chapter III. This report subsection explains rating criteria that the Workgroup developed for the new profiles added to SPECIATE 4.0 and later versions. These ratings are meant to be used for comparing the new profiles relative to one another. In general, the Workgroup believes it is useful to compare a rating based on the number of samples and vintage of the data since profiles created from more tests may be more robust and newer data are more representative of today's emission sources and ever improving measurement techniques. However, one should also consider the J-rating (expert judgment) and NOTES field when selecting profiles for use in their particular application.

The profile ratings developed for the source profiles are based on the following criteria:

- *V-rating (profile vintage)* - the vintage of the profile which reflects measurement technology and methodology. For profiles before year 1980, score = 1; 1980-1990, score = 2; 1991-2000, score = 3; 2001-2005, score = 4; and after year 2006, score = 5. These data are housed in the V_RATING field in the PM and Gas profile tables.

- *D-rating (Data sample size)* - assigned a "1" (poor) to "4" (excellent) rating. This category is rated based on the number of samples: # of samples > 10, score = 4; 5-9 samples, score = 3; 3-4 samples and composite samples, score = 2; 1-2 or unknown # of samples, score = 1. These data are housed in the D_RATING field in the PM and Gas profile tables.

- *Overall Objective Profile Quality Rating* - assigned a value of "A" (highest quality) to "E" (lowest quality) to each non-legacy profile based on the "*Quality Score"* calculated as the "V-rating" x "D-rating". Table 2 shows the range of quality scores that are mapped to each overall profile quality rating. The overall subjective profile quality rating is found in the PM and Gas profile tables under the field named QUALITY.

Table 2. Overall Objective Profile Quality Ratings

Profile Quality	Quality Score Ranges
A	17-20
B	13-16
C	9-12
D	5-8
E	<5

Note that ratings are not provided for the composite profiles since these profiles are developed by combining data for two or more individual profiles that have different scores for the same rating category (see Chapter IV Section M for the description of composite profiles). Also, ratings are not provided for the simplified profiles. The user should refer to the ratings for the individual profiles used to develop the composite and simplified profiles.

Legacy profiles originating from SPECIATE 3.2 do not have entries for V_RATING or D_RATING (or J_RATING shown below); however, they retain their legacy quality rating expressed numerically

(5 = highest quality, 1= lowest quality). The SPECIATE 3.2 documentation does not identify how the quality ratings were selected.

- *J-rating (expert judgment)* - assigned a "1" (poor) to "5" (excellent) rating based on the information underlying each profile, including but not limited to:
    - Profile composition compared with majority of other profiles of the same emission source;
    - Relative ratios of species within the profile;
    - Sum of the speciated mass fractions;
    - Normalization basis (Profiles based on Sum of Species may have only targeted specific compounds and may therefore not be complete.);
    - Supporting documentation;
    - Source of data (e.g. "good" peer-reviewed journals and reports or well-written documents by acknowledged experts in the field); and
    - State-of-the-art data collection and analysis methods used whenever data are obtained.

Many of these items are discussed in more detail in Chapter III. The complexity of each profile precluded the development of an objective rule by which to assign the J-rating. These inherently qualitative values are assigned by the principal investigator for profiles obtained from the Desert Research Institute (DRI), by Abt Associates technical staff, or per the guidance of the Workgroup. EPA SPECIATE workgroup members, DRI and Abt Associates all have extensive experience in source testing for speciation or processing speciated data for emissions inventories, toxic emissions assessment, photochemical modeling, and source-receptor modeling. The technical staff has published numerous peer-reviewed papers and prepared speciation profiles and methodologies for air quality management agencies. Owing to the subjective nature of this rating, J-rating is not a component of the Overall Objective Profile Quality Rating. The overall quality rating and its constituent ratings, as well as the expert judgment rating, are available to the user and auditor for their consideration. Users may consider the ratings as well as the reference and summary information about the profiles housed in the profile tables to determine the suitability of a profile to their needs. Table 3 lists the profile count by J-rating for profiles in SPECIATE 4.5. The distribution of profile J-ratings are shown in Figure 2.

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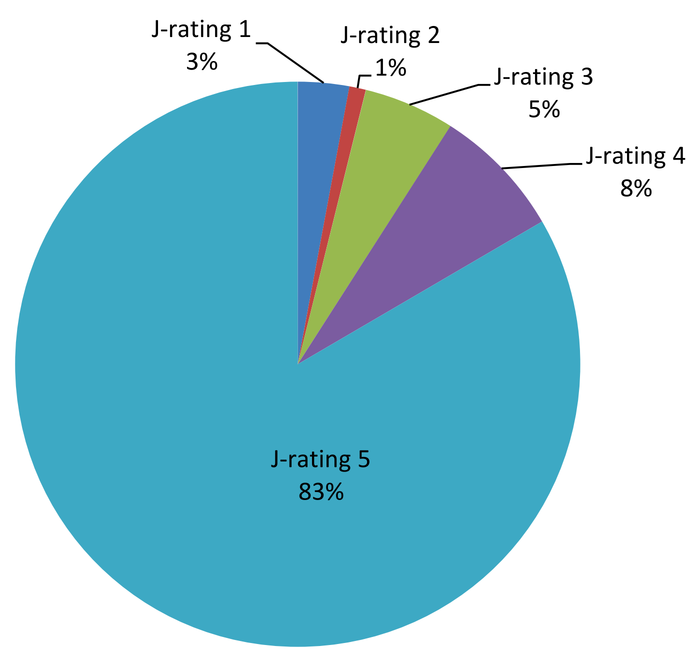
Table 3. Profile Counts by J-rating in the SPECIATE 4.5 Database

	Organic Gas Profiles	PM Profiles	Other Gases Profiles
J-ratings	Counts	Counts	Counts
1	112	2	0
2	29	8	4
3	166	35	2
4	46	238	8
5	1,243	1,768	235

Figure 2. Distribution of Profile J-ratings in SPECIATE 4.5



CHAPTER III. Profiles Included in SPECIATE

Speciation data and profiles obtained from EPA, CARB, DRI, TCEQ, Environment Canada, CRC, NREL, and numerous peer-reviewed journal articles were considered for inclusion in the SPECIATE 4.0 through 4.5 databases.

A list of new speciation profiles added to the SPECIATE 4.5 database, as of June 2016, is shown in Appendix A. Users should refer to the SPECIATE database for the full list of speciation profiles. The following subsections describe significant datasets from which the Workgroup obtained profiles. Subsection A contains new speciation profiles included in the SPECIATE 4.5 database. All other subsections in this chapter identify the profiles carried forward from the SPECIATE 4.0 through 4.4 databases.

During the development of the SPECIATE database, the Workgroup identified hundreds of peer-reviewed journal articles and technical reports to evaluate for use in developing profiles for SPECIATE. The Workgroup prioritized the datasets, with the highest priority given to EPA data as well as the data selected for SPECIATE 4.5 listed in Section A below. The high-priority datasets were further analyzed for completeness of information for profile development, the number of profiles that could be developed, priorities for source categories for which profiles previously were not available or for which improved profiles were needed, and the level-of-effort required to process the datasets. In addition, a MS Excel file (filename is Master Evaluation of Profiles.xlsx) is used to show the prioritization of the datasets and to track the progress of profiles being incorporated into the SPECIATE database. This file contains three worksheets: (1) data completed and incorporated into SPECIATE 4.5; (2) references reviewed that are to be processed for incorporation into future versions of SPECIATE; and (3) reports that do not contain sufficient data or details for developing profiles.

In addition, the Workgroup has prepared guidance to assist profile data collectors on how to collect and present source profile data to maximize their utility to SPECIATE users, to assist future SPECIATE managers in assessing whether the data should be incorporated, and to facilitate the process for preparing profiles in SPECIATE format. This information is provided in Appendix B of this report.

A. New Profiles Included in SPECIATE 4.5

SPECIATE 4.5 includes new profiles from EPA OTAQ, ORD, and Region 8, the U.S. Geological Survey and the scientific literature. EPA’s Office of Transportation and Air Quality continues to develop gasoline, diesel, and natural gas exhaust speciation profiles from onroad and nonroad sources. Other EPA offices (ORD and Region 8) and U.S. Geological Survey have published numerous speciation profiles from oil and natural gas fugitive emissions. Multiple waste incineration and biogenic combustion profiles are identified in the literature as well. The major sources of new profiles that Abt Associates staff incorporated into the SPECIATE 4.5 database are listed below.

1. Speciation Profiles and Toxic Emission Factors for Nonroad Engines (EPA-420-R-14-028; TOG profiles);
2. Assessment of VOC and HAP Emissions from Oil and Natural Gas Well Pads Using Mobile Remote and Onsite Direct Measurement (Brantley et al., 2015; TOG profiles);
3. Tribal Minor Source Registration Data, Region 8 - Uintah & Ouray Indian Reservation (EPA Region 8; TOG profiles);

4. WRAP Phase III oil and gas speciation profiles (WRAP Phase III Support Data; TOG profiles);
5. Petroleum Systems and Geologic Assessment of Oil and Gas in the San Joaquin Basin Province, California (USGS Professional Paper 1713; TOG profiles);
6. VOC Emissions from Oil and Condensate Storage Tanks (Texas Environmental Research Consortium, 2009; TOG profiles)
7. Tunnel studies (Gentner et al., 2013; Liu et al, 2014; NMOG profiles);
8. Animal waste and poultry production (Howard et al., 2010, Trabue et al., 2010; ROG profiles);
9. Gaseous and Particulate Emissions from Prescribed Burning in Georgia (Lee et al, 2005; TOG profiles);
10. Wildland Fire Emissions, Carbon, and Climate: Emission factors (Urbanski, 2014; TOG profiles);
11. Chemical and Physical Characterization of Municipal Sludge Incinerator Emissions (EPA-600/S3-84-047; PM profiles);
12. CNG Transit Bus Exhaust (EPA-420-R-15-022; PM profiles);
13. Carbonaceous Aerosols Emitted from Light-Duty Vehicles Operating on Gasoline and Ethanol Fuel Blends (Hays et al., 2013; PM profiles);
14. Brake wear and tire dust (HEI, Research Report 133 by Schauer et al., 2006; PM profiles);
15. Emissions from Charbroiling and Grilling of Chicken and Beef (McDonald et al, 2003; PM profiles);
16. Oil and Gas Production - Glycol Dehydrator (EPA/OAQPS, 2016; TOG profile); and
17. Natural Gas Flare (EPA/OAQPS, 2016, using TCEQ 2010 Flare Study Final Report).

Other speciation datasets included in SPECIATE 4.5 are light-duty gasoline/diesel exhaust, 2-stroke moped profiles, constituents of fly ash from coal combustion, fireplace and residential wood stove combustion, gas-fired boilers, welding fumes, garbage burning, brick and charcoal making kiln emissions, and composite profiles from oil and natural gas production.

B. Additional EPA Speciation Data

In addition to the above EPA profiles added to the SPECIATE 4.5 database, other EPA data carried forward from previous versions of SPECIATE include the speciation of hundreds of gasoline and diesel liquids and headspace vapors, burning of foliar fuels, agricultural biomass burning, motor vehicle exhaust, iron and steel manufacturing facilities, and oil and natural gas emissions. Examples of major EPA-collected speciation data are provided below:

1. Gasoline and diesel liquids and headspace vapors, and motor vehicle exhaust (EPA, 2008a and 2008b; TOG profiles, added to SPECIATE 4.0, 4.2, and 4.3);
2. Burning of foliar fuels (Hays et al., 2002), agricultural biomass burning (Hays et al., 2005; VOC profiles, added to SPECIATE 4.0);
3. Iron and steel manufacturing facilities (Machemer, 2004; PM profiles, added to SPECIATE 4.0);
4. Combustion of residual fuel oil (Huffman, et al., 2000; PM profiles, added to SPECIATE 4.0);
5. Wood-fired industrial boilers (ERG, 2001; PM profiles, added to SPECIATE 4.0)
6. Exhaust emissions from four-stroke lawn mower engines (Gabele, 1997; TOG profiles, added to SPECIATE 4.2);
7. Heavy-duty vehicle chassis dynamometer testing for emissions inventory, air quality modeling, source apportionment and air toxics emissions inventory (CRC, 2003; CRC, 2005; CRC, 2007; PM and TOG profiles, added to SPECIATE 4.2);
8. Oil-fired utility boilers (Beck, 2004; PM profiles, added to SPECIATE 4.3);

9. Fugitive particulate emissions from construction mud/dirt carryout (Kinsey et al., 2004; PM profiles, added to SPECIATE 4.3);
10. Pulp and paper boilers (EPA, 2003; PM and NMOG profiles, added to SPECIATE 4.3);
11. Physical and chemical characterization of residential oil boiler emissions (Hays et al., 2008; PM and VOC profiles, added to SPECIATE 4.3);
12. Characterization of landfill gas composition at the Fresh Kills municipal solid-waste landfill (Eklund et al., 1998; TOG profiles, added to SPECIATE 4.3);
13. Emissions inventory of $PM_{2.5}$ trace elements across the United States (Reff et al., 2009; PM profiles, added to SPECIATE 4.3);
14. Kansas City PM characterization study (EPA, 2008a; TOG, NMOG, and PM profiles, added to SPECIATE 4.4);
15. Composition of natural gas for use in the oil and natural gas sector rulemaking (EPA, 2011a; TOG profiles, added to SPECIATE 4.4);
16. Composite gasoline headspace vapor - EPAct/V2/E-89 Program and CRC Report CRC-E-80 (EPA, 2009 and CRC, 2011; TOG profiles, added to SPECIATE 4.4);
17. Characterization of carbonaceous aerosols emitted from outdoor wood boilers (Hays et al., 2011; PM profiles, added to SPECIATE 4.4);
18. Hydrocarbon composition of gasoline vapor emissions from enclosed fuel tanks (EPA, 2010 and EPA, 2011b; TOG and VOC profiles, added to SPECIATE 4.4);
19. Emissions from small-scale burns of simulated deployed U.S. military waste (Woodall et al., 2012; VOC profiles, added to SPECIATE 4.4);
20. Chemical characterization of the fine particle emissions from commercial aircraft engines during the Aircraft Particle Emissions eXperiment (APEX) 1 to 3 (Kinsey et al., 2011; PM profiles, added to SPECIATE 4.4); and
21. The effects of operating conditions on semivolatile organic compounds emitted from light-duty, gasoline-powered motor vehicles (Herrington et al., 2012; PM profiles, added to SPECIATE 4.4).

C. Cass Group Speciation Data

Researchers at the California Institute of Technology have conducted many speciation studies. This subsection identifies the studies resulting from this research group for which profiles were developed and included in the SPECIATE database upon recommendation by the Workgroup. Schauer et al. (1998) conducted a research study with CARB to characterize seven air pollution sources: meat charbroiling, cooking with seed oils, medium-duty diesel trucks, gasoline-powered motor vehicles, fireplace combustion of wood, cigarette smoke, and industrial spray painting operations. Along with these seven source sectors, this research study also includes liquid gasoline and headspace vapor profiles and paved road dust profiles for source receptor modeling. Profiles from five out of the seven source sectors are published in peer-reviewed journals. The other profiles mentioned above are identified in the final report to CARB (Schauer et al., 1998) and incorporated into the database.

It is important to note that Schauer et al. continued an earlier CARB funded research study by Rogge, et al. (1993) that applied several techniques to speciate pollutant compositions. Due to limited resources, these profiles have yet to be incorporated into the database.

Both the Schauer et al. and Rogge et al. studies are extremely detailed in that they speciated hundreds of organic compounds in PM, in addition to ions, metals, elemental carbon (EC) and organic carbon (OC). These detailed PM profiles are different from most other PM profiles which usually provide EC, OC, ions, and trace element information only. The additional OC speciation data provide important source markers for receptor modeling (e.g., hopanes, steranes, phenols, syringols, and levoglucosan) and toxic air pollutant (TAP) emission inventories for health risk assessments [e.g., polycyclic aromatic hydrocarbons (PAHs)].

D. California Air Resources Board (CARB) Speciation Profiles

CARB has assembled many TOG and PM profiles as a result of survey work, testing programs, and other research. CARB speciation profiles are available to the public on the internet (CARB, 2003). These profiles are used by CARB during the development of state implementation plans (e.g., to assess photochemical reactivity of VOC mixtures), TAP emission inventories, photochemical modeling, receptor modeling, and other air quality projects. In all, 328 TOG and 8 PM profiles from CARB were selected for incorporation into the SPECIATE database. These profiles cover emission sources such as consumer products (based on 1997 survey data), aerosol coatings (1997 survey data), architectural coatings (1998 survey data), pesticides, landfill gas, wastewater treatment plants, thinning solvents (mineral spirits), degreasing solvents (SPECIATE 4.0), vehicle hot soak (Hsu, 2003; SPECIATE 4.2), and other motor vehicle emission sources powered by California reformulated gasoline (RFG; SPECIATE 4.2).

CARB developed additional profiles as part of CARB funded projects to DRI, and these profiles are included under the DRI data discussion below. Another CARB funded study (CARB, 1991) to speciate organic gas profiles from oil fields in California was added to SPECIATE 4.4.

E. Desert Research Institute (DRI) Speciation Profiles

A total of 1,230 PM speciation profiles were obtained from DRI and incorporated into the SPECIATE 4.0 database. The source sectors represent emissions from geological material, vegetative burning, industrial fuel combustion, forest fires, road dust, refineries, coal combustion, motor vehicles, and many others. Moreover, the profiles measured for the U.S. Department of Energy funded Gasoline-Diesel PM Split Study (DOE, 2005) are included in the SPECIATE 4.2 database.

DRI prepared an additional set of fireplace wood burning and road dust profiles for the California Lake Tahoe Source Characterization Study (Kuhns, et al., 2004), and a study on middle- and neighborhood-scale variations of PM_{10} source contributions in Las Vegas, Nevada (Chow, et al., 1999). Due to priority, these PM profiles will be considered for a later version of SPECIATE.

F. Texas Commission on Environmental Quality (TCEQ) Speciation Profiles

As recommended by the Workgroup, a total of eight VOC profiles for five refineries and three olefin manufacturing plants were added to the SPECIATE 4.0 database (Allen, 2004). However, these profiles are given a low quality rating because metadata (e.g., analytical and sampling methods, source documentation, number of samples needed for profile quality rating) are not readily available and significant resources would be required to retrieve the underlying information (i.e., reviewing the facility reports, likely maintained at the facilities).

G. Profiles Prepared from Environment Canada's National Pollutant Release Inventory

A total of 100 VOC profiles were developed and included in the SPECIATE 4.1 database (and carried forward in later versions of SPECIATE) from data contained in Environment Canada's National Pollutant Release Inventory (NPRI). The NPRI is the only nationwide, publicly-accessible program of its type in Canada that provides information on annual releases of pollutants to the air, water, land, and disposal or recycling from all sectors.

The NPRI database contains 22 tables that are structured in an MS Access relational database format. The NPRI database provides detailed stationary source facility-level emissions by pollutant along with facility contact information, addresses, and North American Industry Classification System (NAICS) code and/or Canadian or American Standard Industrial Classification (SIC) code. For this project, several methods were developed to match the fields in the NPRI database to the format of SPECIATE. The main difference between the SPECIATE database and the NPRI database is that the NPRI data are not provided at the emissions process or unit level but are aggregated to the facility level to avoid the disclosure of confidential information. Consequently, many of the data fields in the two databases could not be matched directly. For example, a facility may have emissions from boilers fueled with diesel and natural gas, volatile compound emissions from fugitive sources, and emissions from internal combustion engines. All of these speciated emissions are collectively registered to one facility account in the NPRI database by plant operators. Since operation of each emission source is different from one plant to another, the SPECIATE database is designed to capture speciation profiles in the most disaggregated form possible.

H. Environment Canada Mobile Source Speciation Profiles

In addition to the NPRI database, Environment Canada also has extensive research programs to characterize emissions from vehicles with various engine and emission control technologies when operated on traditional gasoline, different blends of ethanol gasolines, diesel, biodiesel, and other fuels. Several studies tested vehicles at 0 ^{o}C and 20 ^{o}C for speciated emission composition comparisons (e.g., ERMD Report 00-37). Programs were undertaken to help identify and quantify the emissions impact of different blended fuels on the tailpipe and evaporative emissions. In general, reports discuss gaseous emissions of carbon monoxide (CO), oxides of nitrogen (NO_x), total hydrocarbon (THC), non-methane hydrocarbons (NMHC), non-methane organic gases (NMOG), ethanol, and PM, in addition to comprehensive speciated compounds (e.g., ERMD Report 1998-26718, ERMD Report 2005-39; SPECIATE 4.2).

I. Coordinating Research Council E-75 Diesel Exhaust Speciation Database

In order to better assess the current state of speciated diesel emissions data, the CRC and the U.S. DOE NREL jointly contracted with consultants to conduct the E-75 project comprising the following three objectives:

- Perform a literature review of diesel speciation studies;
- Compile speciated exhaust emissions data from on-road diesel vehicles designed to meet U.S. emission standards; and
- Assess the quality and completeness of the data.

The consultants reviewed studies that provided data on speciated diesel exhaust emissions from vehicles with and without the use of advanced emission reduction technologies. In performing the literature search to determine the datasets that could be incorporated into a diesel emissions database for this project, the consultants accessed peer-reviewed materials such as journal papers [e.g., Environmental Science and Technology (ES&T)] and papers and reports from the Society of Automotive Engineers, CRC, NREL, CARB, U.S. EPA, and research institutes (e.g., University of Wisconsin, West Virginia University, University of California at Riverside)]. After review and analysis of the report content and speciation methodology employed, the consultants summarized the suitability of each reference for this project (Hsu and Mullen, 2007). Multiple heavy duty diesel exhaust profiles have been incorporated into the SPECIATE database (SPECIATE 4.2 and 4.3).

J. SPECIATE 3.2 Legacy Profiles

The profiles in SPECIATE 3.2 have been incorporated into SPECIATE 4.0 and carried forward in later database versions. The GAS_PROFILE and PM_PROFILE tables in the SPECIATE 4.5 database both contain a field named VERSION to identify profiles that originate from SPECIATE 3.2 (see Table 1 for the definition of this field). The data from SPECIATE 3.2 are reformatted for storage in the SPECIATE 4.5 database, but the additional fields that appear in SPECIATE 4.5 and not in SPECIATE 3.2 are not populated. The SPECIATE 3.2 profiles are not subject to the SPECIATE 4.5 profile rating criteria as discussed in Chapter II.

CHAPTER IV. Important Notes and Comments Related to the SPECIATE Database

Throughout this project, the Workgroup raised issues and questions regarding the SPECIATE database. This chapter describes results and recent decisions made by the Workgroup.

A. Completeness of the SPECIATE Database

The SPECIATE 4.5 database includes speciation profiles covering the top 20 VOC and PM contributing source sectors in the 2011 NEI, accounting for over 80% of all emissions. For example, EPA constructed VOC and PM foliar fuel profiles that are appropriate to the prescribed burning and wildfires categories, two of the largest VOC and PM emission sectors in the NEI. There are also TOG profiles for oil and gas extraction fugitive emissions, natural gas flaring, gasoline motor vehicle exhaust (catalyst and non-catalyst), surface coatings (architectural coatings and aerosol coatings both solvent-borne and water-borne), liquid gasoline and the latest EPA gasoline exhaust, evaporative, and diesel headspace profiles all reflect changes in new regulations and formulations. A much more complete speciation of diesel exhaust VOC is also included in the SPECIATE 4.5 database. The gasoline and diesel onroad sectors are among the largest organic gas emitters.

Speciation data for other large emission sectors like paved and unpaved road dust, degreasing, diesel exhaust, pesticides, solvents, consumer products, fireplaces, dry cleaning, graphic arts and household products were included in SPECIATE 4.4 and carried forward into the SPECIATE 4.5 database.

During the development of the SPECIATE 4.5 database, the Workgroup identified many mobile source emissions datasets that contain diesel exhaust PM and organic gases, gasoline vehicle exhaust and evaporative emissions, and non-road vehicle emissions. In addition to conventional vehicle emissions data, future fuels (e.g., low sulfur diesel, biodiesel), and advanced technology vehicles are included in the SPECIATE 4.5 database.

Even though SPECIATE 4.5 contains speciation profiles for a comprehensive list of emission sources, the Workgroup continuously strives to search for speciation data that are more specific for source types, processes, and different regions. Examples of source sectors where speciation data profiles are needed include the oil and gas industry (extraction wells, dehydration sumps, processing plants, storage tanks, distribution and transmission leaks), household and yard waste burning, biodiesel engine exhaust, pulp and paper industry boiler combustion, architectural and industrial maintenance coating, wild fires, prescribed burnings, and coal-fired power plants. There are also data gaps for PM profiles that differentiate filterable and condensable speciation data. In addition to individual profiles, composite profiles are also important for SPECIATE users.

B. Unresolved Mixtures within Profiles

Many TOG and VOC speciation profiles contain mixtures of compounds listed as a single species (e.g., surface coatings and adhesives profiles have mineral spirits and/or “aromatic 100” solvents). Users could further speciate these unresolved fractions using appropriate solvent profiles provided in the SPECIATE 4.5 database (i.e., organic gas profile numbers 3141 and 4423 - 4461). Further effort should be expended to resolve these mixtures within each of the SPECIATE profiles. This is an important issue for many users of SPECIATE, including photochemical modelers, inventory preparers, and control strategy analysts.

Photochemical modelers have expressed an interest in seeing these mixtures resolved in speciation profiles (Carter, 2004).

The issue of unresolved mixtures is illustrated in Table 4 below using the example TOG profile #2425 for "surface coatings – general". The top chemical listed is mineral spirits at 31% by weight. Another important mixture in this profile is xylene isomers at 11% by weight. Since these chemicals are made up of many individual species, the use of this profile can present problems for users. Speciation profiles for mineral spirits and xylene mixtures are shown in Appendix C. Additional effort is needed to resolve the mixtures in order to present reasonably complete (i.e., species-specific) profiles for the user community. The key profiles are those with substantial amounts of mixtures (e.g., >3-5% by weight) and those that are commonly used in regional modeling and inventory development. For example, although there are additional mixtures shown in the profile in Table 4 (e.g., oxygenates, ketones), their contributions are fairly small.

Table 4. Profile #2425 for Surface Coatings - General

Chemical Name	Weight Percent	CAS#
MINERAL SPIRITS	31.05	64475850
TOLUENE	12.34	108883
XYLENE, ISOMERS OF	11.02	1330207
METHYL ETHYL KETONE	4.16	78933
BUTYL ACETATE N-	3.90	123864
ETHYLENE GLYCOL	3.35	107211
METHYL ISOBUTYL KETONE	3.15	108101
BUTYL CELLOSOLVE	2.94	111762
DIACETONE ALCOHOL	2.94	123422
BUTYL ALCOHOL S-	2.92	78922
ACETONE	2.36	67641
ISOBUTYL ALCOHOL	2.06	78831
ETHYL ALCOHOL	1.69	64175
ETHYL ACETATE	1.50	141786
ISOPROPYL ALCOHOL	1.50	67630
PROPYLENE GLYCOL	1.24	57556
TRICHLOROETHANE 1,1,1-	1.01	71556
UNDEFINED VOC	0.87	
PROPYL ACETATE N-	0.60	109604
PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	0.60	108656
BUTYL CARBITOL	0.54	112345
OXYGENATES	0.49	
KETONES – GENERAL	0.44	
CELLOSOLVE ACETATE	0.36	111159
METHOXY-2-PROPANOL 1-	0.30	107982
MONOMETHYL ETHER DIPROPYLENE GLYCOL	0.30	34590948
CELLOSOLVE	0.24	110805
CARBITOL	0.12	111900
METHYL CARBITOL	0.12	111773

The profiles listed for mineral spirits and xylene mixtures in Appendix C show that there are important implications for resolving these mixtures. For users involved in preparing TAP inventories, important species are present in significant amounts (e.g., toluene, ethylbenzene, xylene isomers). Resolving these mixtures will also help photochemical modelers and control strategy analysts better understand the reactivity of the overall profile.

C. Preference of New Profiles

For certain source categories, SPECIATE users can choose from a set of relevant profiles. The SPECIATE 4.5 database incorporates updated speciation profiles that reflect the changes in product composition that have been made in response to new regulations (e.g., ethanol blended gasoline) and sampling technologies (e.g., dilution sampling for combustion sources). For example, consumer and commercial product categories are among the highest contributors to VOC emissions nationally. Due to new federal and state regulations, different ingredients have been developed for consumer products. Users should take into account the most appropriate vintage of profile for their particular application. Another example is the reduction of lead content in road dust, presumably due to the phase-out of leaded gasoline. Newer profiles are generally recommended where a choice exists, except when conducting retrospective emissions or modeling analyses. Therefore, users should refer to the TEST_YEAR field associated with each profile when choosing profiles. The V_RATING field may also be useful for this purpose.

D. Identification of Species

The individual species that make up the profiles may be identified by several methods, so the SPECIATE 4.5 database provides several fields that can be used to distinguish each species. A Chemical Abstracts Service (CAS) number is an identifier assigned to a specific compound by the American Chemical Society (ACS). EPA is often interested in groups of compounds, such as VOCs or PAHs. These groups are assigned EPA IDs where there are no CAS numbers in ACS. CAS numbers and EPA IDs are mutually exclusive -- that is, a compound or group never has both identifiers. An EPA internal tracking number (ITN) is assigned to all compounds or groups tracked in the EPA Substance Registry System (SRS) and makes a useful unique identifier for compounds/groups. However, it is not as well-known or as readily available as the CAS number. Finally, ongoing research and analysis shows that there are compounds and mixtures that have no associated identification numbers.

Within the SPECIATE 4.5 database, all species, whether individual compounds or groupings, are identified and detailed in the SPECIE_PROPERTIES table. A unique Species ID is designated for each species tracked within the database; its various identifiers and characteristics are stored in the fields or columns of the record. The internal workings of SPECIATE depend on the Species ID within the SPECIATE 4.5 database, rather than a particular ID number (such as CAS or EPA ID). Thus, the SPECIATE 4.5 database can function with or without the presence of a CAS or EPA ID.

In cases where neither the CAS number, EPA ID, nor EPA ITN is available, the ID field in the SPECIE_PROPERTIES table may be used to identify species in ancillary applications, such as mappings. Note that the SPECIATE temporary ID was used during the development of SPECIATE 4.0 to facilitate tracking of data but is no longer used.

If a CAS number, EPA ID, or EPA ITN is subsequently defined for a compound or group, that information will be recorded in the SPECIATE database in the SPECIE_PROPERTIES table. The EPA Office of Environmental Information provided identification information on compounds in SPECIATE that were previously without identification numbers and are tracked in the SRS. These identifiers have been incorporated into the SPECIATE 4.5 database in the SPECIE_PROPERTIES table.

SAROAD codes are the other widely used chemical identifiers. However, EPA no longer maintains SAROAD codes for chemicals. Currently, SAROAD codes are included in many speciation databases and are built into photochemical and dispersion models. Since there is no central SAROAD codes database, there are several versions of SAROAD codes among EPA, state agencies and organizations (due to users generating their own SAROAD codes, as needed). Since there are conflicts in SAROAD codes, the Workgroup is undecided about whether they should be included in the SPECIATE database. For SPECIATE 4.5, the SAROAD codes associated with SPECIATE 3.2 profiles are kept in the database.

E. Mass Fractions of Unmeasured Species

To account for as much as possible of the emitted mass of fine particulate matter ($PM_{2.5}$), Reff et al. (2009) calculated additional species that were not in the original raw profiles in SPECIATE. Details about these calculations are provided below.

Particulate-Bound Water

Reff et al. (2009) calculated particulate-bound water (H_2O) emissions for each composite profile as 24% of the sum of $SO_4^{=}$ and NH_4^{+} emissions. H_2O emissions from combustion and other high-temperature sources were forced to be 0 with the expectation that the water emitted from such environments is likely to be in the vapor phase. Sources considered to have no particulate H_2O emissions are agricultural burning, bituminous combustion, calcium carbide furnace, charbroiling, charcoal manufacturing, distillate oil combustion, electric arc furnace, ferromanganese furnace, glass furnace, heavy-duty diesel vehicle (HDDV) exhaust, heat treating, Kraft recovery furnace, light-duty diesel vehicle (LDDV) exhaust, lignite combustion, lime kiln, meat frying, natural gas combustion, non-road gasoline exhaust, on-road gasoline exhaust, open hearth furnace, prescribed burning, process gas combustion, pulp & paper mills, residential coal combustion, residential natural gas combustion, residential wood combustion, residual oil combustion, sintering furnace, slash burning, sludge combustion, solid waste combustion, sub-bituminous combustion, wildfires, and wood fired boilers.

Metal-Bound Oxygen

Reff et al. (2009) calculated metal-bound oxygen (MO) by multiplying most of the trace elemental emissions by an oxygen-to-metal ratio. These ratios were based on the expected oxidation states of the metals in the atmosphere. Table 5 shows the expected oxide forms of each metal, which are based on the most common oxidation states of the metals. Total MO was then calculated for each source category using the following equation:

$$MO = \sum_{El}^{n} Ox_{El} \cdot E_{El}$$

where O_{xEl} is the oxygen-to-metal ratio for metal *El*, and E_{El} is the emission of metal *El* after accounting for bonding with $SO_4^{=}$. For metals with more than one common oxidation state, the mean of the oxygen-to-metal ratios was used for the O_{xEl} value (see Table 5).

Table 5. Assumed Oxide Forms of Each Metal and Resulting Mean Oxygen-to-Metal Ratio Used to Calculate the Emissions of Metal-Bound Oxygen

Species	Oxide Form 1	Oxide Form 2	Oxide Form 3	Oxygen/Metal Ratio
Na	Na_2O			0.348
Mg	MgO			0.658
Al	Al_2O_3			0.889
Si	SiO_2			1.139
P	P_2O_3	P_2O_5		1.033
K	K_2O			0.205
Ca	CaO			0.399
Ti	TiO_2			0.669
V	V_2O_5			0.785
Cr	Cr_2O_3	CrO_3		0.692
Mn	MnO	MnO_2	Mn_2O_7	0.631
Fe	FeO	Fe_2O_3		0.358
Co	CoO	Co_2O_3		0.339
Ni	NiO			0.273
Cu	CuO			0.252
Zn	ZnO			0.245
Ga	Ga_2O_3			0.344
As	As_2O_3	As_2O_5		0.427
Se	SeO	SeO_2	SeO_3	0.405
Rb	Rb_2O			0.094
Sr	SrO			0.183
Zr	ZrO_2			0.351
Mo	MoO_2	MoO_3		0.417
Pd	PdO	PdO_2		0.226
Ag	Ag_2O			0.074
Cd	CdO			0.142
In	In_2O_3			0.209
Sn	SnO	SnO_2		0.202
Sb	Sb_2O_3	Sb_2O_5		0.263
Ba	BaO			0.117
La	La_2O_3			0.173
Ce	Ce_2O_3	CeO_2		0.2
Hg	Hg_2O	HgO		0.06
Pb	PbO	PbO_2		0.116

This is an extension of the assumption described by Malm et al. (1994), where two common forms of Fe are assumed to exist in ambient particulate matter in equal quantities. The list of metal oxides in Table 5 is inclusive of metal oxide forms used in some previous studies of particulate matter. In the Sea Salt profile, MO is forced to be zero because the Na, Mg, Ca, and K ions are assumed to be neutralized by Cl^- and $SO_4^=$ rather than oxygen. In the Agricultural Burning profile, the Workgroup assumed all K to be in the form of KCl rather than K_2O.

Particulate Non-Carbon Organic Matter

Particulate Non-Carbon Organic Matter (PNCOM) consists of hydrogen, oxygen, nitrogen, and other elements bound to carbon in OC. PNCOM is calculated for each source category by multiplying OC emissions by a source-category specific organic matter (OM)/OC ratio to calculate an OM emission, and subtracting OC from OM. For all new profiles added to SPECIATE 4.5 in 2016, we used the methods described in Reff et al. (2009) unless PNCOM was explicitly measured and reported in the source tests.

Reff et al. (2009) used an OM/OC ratio of 1.25 for all motor vehicle exhaust sources (LDDV and HDDV exhaust, non-road and on-road gasoline exhaust source categories), which is a median of the values from Aiken et al. (2008) (1.22, 1.25); Lipsky and Robinson (2006) with artifact correction (1.4); Russell (2003) (1.2, 1.3, 1.1); and Japar et al (1984) (1.43). This ratio is also fairly consistent with the value of 1.2 used by Kleeman et al. (2000) and Sheesley et al. (2003), based on the measurements by Schauer et al. (1999, 2002).

Reff et al. (2009) used an OM/OC ratio of 1.7 for wood combustion sources (wildfires, agricultural burning, residential wood combustion, prescribed burning, and slash burning source categories), which is a median of the values from Aiken et al. (2008) (1.55, 1.7); Lipsky and Robinson (2006) with artifact correction (1.8); Hays et al. (2002) (1.2); and Turpin and Lim (2001) (1.9) – the 1.9 was computed from the organic-molecular data of Schauer et al. (2001). The ratio of 1.7 is in agreement with the mass-closure estimates reported by Sheesley et al. (2003) (1.7) and Bae et al. (2006) (1.74), and falls in the range of estimates reported by Jimenez et al. (2007) (1.5, 1.8, and 2.0). The Wood Fired Boiler category was originally assigned an OM/OC ratio of 1.7, but was changed from 1.7 to 1.4 because a wood-fired boiler should not have as much oxygen as an open fire (Reff et al., 2009).

An OM/OC ratio of 1.4 was applied to the emissions from all other source categories based on the long-standing value used in numerous studies of atmospheric $PM_{2.5}$ (Turpin and Lim, 2001).

Ammonium

In cases where NH_4^+ values were not explicitly measured, NH_4^+ values were imputed stoichiometrically in the profiles for the Ammonium Sulfate Production [assuming $(NH_4)_2SO_4$] and Ammonium Nitrate Production (assuming NH_4NO_3) source categories.

Sulfate and Sulfur

Many of the raw profiles contained a value for either $SO_4^=$ or S, but not both. In these cases, Reff et al. (2009) used stoichiometry to compute the missing value from the available measurement (assuming all S was present in the form of $SO_4^=$). In profiles of the Ammonium Sulfate Production, Copper Processing, Lime Kiln, and Catalytic Cracking categories, both $SO_4^=$ and S values were given in the data, but they were not stoichiometrically consistent. In these cases S was computed from $SO_4^=$ due to the higher accuracy of ion chromatography compared to X-ray fluorescence.

F. Renormalization of PM Profiles

Most PM profiles are normalized to the gravimetric mass of PM by dividing the species weight by the gravimetric mass of PM collected on Teflon filters as reported in the primary literature. Due to the nature of sampling and analytical technologies, many PM speciation profiles show a total mass of larger than 100% due to OC measurements having "organic gas adsorption artifacts". OC collected on quartz fiber filters have positive artifacts due to adsorption of organic gases on the filter. Desorption of SVOC contributes to negative artifacts. There is no easy fix for these artifacts (Chow, 2004). Organic gas denuders and backup quartz fiber filters have been studied as methods for correcting these artifacts, but there are no standard solutions to date. Most of these profiles are technically accurate for the individual components.

DRI applied two other normalization bases to a set of DRI PM profiles (SPECIATE 4.0). When measured mass was below 1 to 2 milligrams (mg) or exceeded 5 mg, the effect of gaseous OC adsorption on quartz-fiber filters became apparent since the sum of the ratio of chemical species to measured mass ratios exceeded unity. These samples were renormalized to the sum of species or reconstructed mass rather than measured gravimetric mass. For the sum of species, only total carbon (TC) was used to represent carbonaceous material while $1.4 \times [OC] + [EC]$ was used for reconstructed mass to account for the mass of other elements (such as N, S, and O) associated with OC. The factor of 1.4 was selected to adjust the OC mass for other elements assumed to be associated with the OC molecule (White and Roberts, 1977; Japar et al., 1984). Similarly, crustal material was estimated by $2.2 \times [Al] + 2.49 \times [Si] + 1.63 \times [Ca] + 2.42 \times [Fe] + 1.94 \times [Ti]$ in the reconstructed mass by summing the mass of those elements predominantly associated with soil, with allowance for oxygen present in the common compounds (e.g., Al_2O_3, SiO_2, CaO, K_2O, FeO, Fe_2O_3, TiO_2). The NORM_BASIS field in the PM_PROFILE table identifies the normalization basis (PM mass, sum of species, or reconstructed mass) used for a DRI profile if this information is available.

To compute "model-ready" PM profiles, new speciation profiles added to SPECIATE 4.5 in 2016 (i.e., 95219, 95220, 95429 – 95462) are normalized by reconstructed mass using the method laid out in Reff et al. (2009). The reconstructed mass is calculated by summing the mass of speciated compounds (e.g., EC, OC, metals) and those inferred (e.g., particulate-bound water, MO, and PNCOM). When the reconstructed mass is less than the PM gravimetric mass, an additional species called "Other Unspeciated PM" is added to the profile to make the sum of species equal to 100% of PM. In this case, the gravimetric mass of PM is applied to normalize the profile.

G. Avoiding Double-Counting Compounds

The total speciated percentage of a given PM profile is listed under the TOTAL field in the SPECIATE 4.5 database. It is calculated as the sum of all speciated compounds (e.g., EC, OC, sulfates, nitrates, metals), excluding elemental sulfur and speciated organics in PM (e.g., PAHs).

As described previously, speciated organic compounds are measured in many of EPA's and Schauer's PM profiles. The mass of these organic species is divided by PM mass to calculate their mass fraction. For these PM profiles, the mass of each PM-associated organic species is excluded from the sum of all speciated compounds to avoid double-counting with OC and PNCOM (i.e., organic species such as PAHs are included in the OC and PNCOM fractions). The OC included in these PM speciation data have a higher mass than the sum of the speciated organic compounds (since not all species are identified and quantified). Therefore, the

OC mass is used in the calculation of total PM mass when the profile is developed in order to achieve better mass closure.

Similarly, elemental sulfur and ionic sulfate are measured in many PM speciation datasets. They are analyzed using different analytical techniques (e.g., X-ray fluorescence spectroscopy, flame atomic absorption, ion chromatography). For the purposes of determining total PM mass, the ionic sulfate results from the ion chromatography analysis are used, since this technique provides a higher total mass than the elemental measurements.

H. Inorganic Gases in PM Profiles

Sulfur dioxide, ammonia and other inorganic gases are sometimes collected and measured along with DRI PM. Sulfur dioxide and other gases are presented as percentages by dividing the individual gas mass by total PM mass but are not included in the Total Mass calculation for the profile. The Workgroup recommended inclusion of inorganic gases for receptor modeling purposes, with inorganic gases distinctly indicated as a gas in the chemical names. Inorganic gases are not added to the PM mass. The database includes a field (INCL_GAS) indicating whether a PM profile has associated inorganic gases. These DRI PM profiles were added to SPECIATE 4.0 database and carried forward into the SPECIATE 4.5 database.

I. Correction Factors for Oxygenated Compounds

The EPA gasoline and diesel headspace vapor data are calibrated by generic standards (e.g., correlate gas chromatograph responses to hexane standard gas), and, therefore, need to be adjusted with correction factors (Lewis, 2004). Common oxygenated compounds in speciation profiles are ethanol, methyl t-butyl ether (MTBE), and t-amylmethyl ether (TAME). The mass percentages for oxygenated compounds are adjusted based on gas chromatography responses. These oxygenated compounds are adjusted based on correction factors in the literature (1.5, 1.25, and 1.2 for ethanol, MTBE, and TAME, respectively; Scanlon et al., 1985; Jorgensen et al., 1990). Both adjusted and unadjusted speciation profiles for the EPA headspace vapor data are incorporated in SPECIATE 4.0 database and carried forward into SPECIATE 4.5. The terms “adjusted for oxygenates” and “not adjusted for oxygenates” are added to the end of the names of the profiles in the GAS_PROFILE table in the SPECIATE 4.5 database to clearly identify the profiles for which response factors are applied versus the profiles for which the response factors are not applied.

J. Other Correction Factors

Thermal optical reflection (TOR) and thermal optical transmission (TOT) instruments are commonly used to measure EC and OC. Both analyzers quantify carbon atoms only (i.e., the mass of associated oxygen, hydrogen, nitrogen and other atoms is not included). EC and OC measurements reported in DRI PM profiles are measured by the TOR procedure. EPA and Schauer’s profiles used the TOT procedure for EC and OC analyses. This is important since previous studies have observed that the discrepancy in EC resulting from TOR and TOT procedures could be up to 40% due to differences in the operational definitions of EC and OC. Since there is no consensus on the best method for EC and OC measurements, data are reported as measured without an adjustment. The SPECIATE 4.5 database includes an analytical methods field (ANLYMETHOD) in the PM_SPECIE table indicating which method is used.

K. Data from Tunnel Studies

Profiles generated from tunnel studies should be associated with onroad motor vehicle emissions, including mixtures of gasoline and diesel exhaust, evaporative sources, road dust, tire wear, brake wear, etc. These types of profiles can be identified from references in the database as well as the NOTES field. While these types of profiles may not be useful for the purposes of emission inventory development (since they are mixtures of many emission sources), they are useful for source apportionment (receptor) modeling.

L. VOC-to-TOG Conversion Factors

The process of calculating the VOC-to-TOG conversion factor for a given profile consists of determining the organic gases in the profile that are exempted from the EPA VOC definition and determining what portion of the overall profile is composed of these non-photochemically reactive compounds (e.g., methane, ethane, acetone). Once the weight fraction sum of these non-photochemically reactive compounds is known, it is divided into 1 to obtain the VOC-to-TOG conversion factor. The EPA definition of VOC and a list of exempt organic gases are available at http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8 (accessed June 2016).

Using the EPA list of exempt organic gases, database queries are used to compute the VOC-to-TOG conversion factors. For example, if a profile contains 20% methane (not a VOC) and 80% VOC, the VOC-to-TOG conversion factor is the sum of all species divided by the portion that is VOC, or 100 ÷ 80 in this example. The resulting conversion factor (1.25) is stored with the profile in the VOC to TOG field. It can be applied to an estimate of VOC emissions to estimate TOG emissions. For composite profiles, the conversion factors are computed after the composites are developed.

M. Composite PM and TOG Profiles

Many emission source categories have multiple speciation profiles in prior SPECIATE versions. There are 131 composite PM profiles (Reff et al., 2009) carried forward into the SPECIATE 4.5 database. There are four composite tire dust and brake wear PM profiles (95495 – 95462) added to SPECIATE 4.5. Table 6 lists the P_NUMBER and name of the profiles. Users may employ the composite profiles to avoid manual comparison of several relevant but diverse profiles, using the Workgroups as an indication of central tendency for the source category. Users may equally prefer their own analysis of the constituent profiles, determining the best fit for their needs, thereby obviating the need for the composites.

The PM-composite profiles developed by Reff et al. (2009) are identified by profile numbers (P_NUMBER) that start with "91xxx". The term "composite" is also included at the end of the name in the NAME field in the PM_PROFILE table. The composite profiles are easily identified by the ORIG_COMPO field (allowed value = "O" for Original, "C" for Composite, Null for legacy profiles). The NOTES field in the PM_PROFILE table identifies the individual profiles (first included in the SPECIATE 4.2 database) upon which the composite profiles are based. The documentation provided in the NOTES field is also provided in the DESCRIPTION field in the REFERENCE table; the DOCUMENT field in the REFERENCE table is null since the composite profiles are based on more than one individual profile. Users may look-up the references for the individual profiles in the database to identify the references supporting the PM-composite profiles.

Table 6. PM Composite Profiles Carried Forward into the SPECIATE 4.5 Database

P_NUMBER	NAME
91000	Draft Agricultural Burning - Composite
91001	Draft Agricultural Soil - Composite
91002	Draft Brake Lining Dust - Composite
91003	Draft Catalytic Cracking - Composite
91004	Draft Cement Production - Composite
91005	Draft Charbroiling - Composite
91006	Draft Cigarette Smoke - Composite
91007	Draft Construction Dust - Composite
91008	Draft Copper Production - Composite
91009	Draft Crustal Material - Composite
91011	Draft Electric Arc Furnace - Composite
91012	Draft Ferromanganese Furnace - Composite
91013	Draft Fly Ash - Composite
91014	Draft Food & Ag - Handling - Composite
91015	Draft Industrial Soil - Composite
91016	Draft Inorganic Fertilizer - Composite
91017	Draft LDDV Exhaust - Composite
91018	Draft Lime Kiln - Composite
91019	Draft Limestone Dust - Composite
91020	Draft Natural Gas Combustion - Composite
91021	Draft Non-catalyst Gasoline Exhaust - Composite
91022	Draft Onroad Gasoline Exhaust - Composite
91023	Draft Paved Road Dust - Composite
91024	Draft Phosphate Manuf - Composite
91025	Draft PMSO2ControlledLigniteCombustion - Composite
91026	Draft Prescribed Burning - Composite
91027	Draft Process Gas Combustion - Composite
91028	Draft Residential Coal Combustion - Composite
91029	Draft Residential Wood Combustion: Eucalyptus - Composite
91030	Draft Residential Wood Combustion: Hard - Composite
91031	Draft Residential Wood Combustion: HardSoft - Composite
91032	Draft Residential Wood Combustion: HardSoftN/A - Composite
91033	Draft Residential Wood Combustion: Soft - Composite
91035	Draft Sand & Gravel - Composite
91036	Draft Sandblast - Composite
91037	Draft Secondary Aluminum - Composite
91038	Draft Sintering Furnace - Composite
91039	Draft Slash Burning - Composite
91040	Draft Solid Waste Combustion - Composite
91041	Draft Sub-bituminous Combustion - Composite

P_NUMBER	NAME
91042	Draft Surface Coating - Composite
91043	Draft Tire Dust - Composite
91044	Draft Unpaved Road Dust - Composite
91045	Draft Wildfires - Composite
91046	Draft Wood Product Drying - Composite
91047	Draft Wood Product Sawing - Composite
91048	Draft Bituminous Coal Combustion - Composite
91100	Unpaved Road Dust - Composite
91101	Agricultural Soil - Composite
91102	Wildfires - Composite
91103	Agricultural Burning - Composite
91104	Bituminous Combustion - Composite
91105	Residential Wood Combustion - Composite
91106	HDDV Exhaust - Composite
91107	Construction Dust - Composite
91108	Paved Road Dust - Composite
91109	Prescribed Burning - Composite
91110	Sub-bituminous Combustion - Composite
91111	Sand & Gravel - Composite
91112	Natural Gas Combustion - Composite
91113	Nonroad Gasoline Exhaust - Composite
91114	Wood Fired Boiler - Composite
91115	Distillate Oil Combustion - Composite
91116	Charbroiling - Composite
91117	Residual Oil Combustion - Composite
91118	Dairy Soil - Composite
91119	Kraft Recovery Furnace - Composite
91120	Mineral Products - Avg - Composite
91121	Industrial Manufacturing - Avg - Composite
91122	Onroad Gasoline Exhaust - Composite
91123	Heat Treating - Composite
91124	Chemical Manufacturing - Avg - Composite
91125	Lignite Combustion - Composite
91126	Solid Waste Combustion - Composite
91127	Cement Production - Composite
91128	Wood Products - Drying - Composite
91129	Surface Coating - Composite
91130	Food & Ag - Handling - Composite
91131	Wood Products-Sawing - Composite
91132	Aluminum Processing - Composite
91133	Open Hearth Furnace - Composite
91134	Brake Lining Dust - Composite

P_NUMBER	NAME
91135	Meat Frying - Composite
91136	Process Gas Combustion - Composite
91137	Aluminum Production - Composite
91138	Lime Kiln - Composite
91139	Sintering Furnace - Composite
91140	Charcoal Manufacturing - Composite
91141	Catalytic Cracking - Composite
91142	Fiberglass Manufacturing - Composite
91143	Glass Furnace - Composite
91144	Pulp & Paper Mills - Composite
91145	Petroleum Industry - Avg - Composite
91146	Slash Burning - Composite
91147	Misc. Sources - Composite
91148	Asphalt Roofing - Composite
91149	Inorganic Chemical Manufacturing - Composite
91150	Tire Dust - Composite
91151	Ferromanganese Furnace - Composite
91152	Wood Products - Sanding - Composite
91153	Electric Arc Furnace - Composite
91154	Food & Ag-Drying - Composite
91155	Residential Coal Combustion - Composite
91156	Residential Natural Gas Combustion - Composite
91157	Cast Iron Cupola - Composite
91158	Copper Processing - Composite
91159	Asphalt Manufacturing - Composite
91160	Fly Ash - Composite
91161	Sandblast - Composite
91162	LDDV Exhaust - Composite
91163	Ammonium Nitrate Production - Composite
91164	Limestone Dust - Composite
91165	Phosphate Manufacturing - Composite
91166	Gypsum Manufacturing - Composite
91167	Urea Fertilizer - Composite
91168	Lead Processing - Composite
91169	Crustal Material - Composite
91170	Copper Production - Composite
91171	Brick Grinding and Screening - Composite
91172	Calcium Carbide Furnace - Composite
91173	Coke Calciner - Composite
91174	Industrial Soil - Composite
91175	Potato Deep Frying - Composite
91176	Sea Salt - Composite

P_NUMBER	NAME
91177	Sludge Combustion - Composite
91178	Lead Production - Composite
91179	Steel Desulfurization - Composite
91180	Auto Body Shredding - Composite
91181	Ammonium Sulfate Production - Composite
91182	Inorganic Fertilizer - Composite
91183	Boric Acid Manufacturing - Composite

The weight percent value of each species included in the composite profile is based on the median weight percent value available from the individual profiles upon which the composite profile is based. For some source categories (e.g., paved road dust), composite profiles are created hierarchically by forming a "subcomposite" profile based on profiles that are measured from very similar source tests (e.g., Central California road dust) and then computing a composite based on the median of the subcomposite profiles. The median is chosen over the mean to help mitigate possible large errors stemming from the presence of outlier samples and measurements (Reff et al., 2009). Null values in the individual profiles are treated as "no data available" and are excluded from determining the median value for the composite profile. Zero values in the individual profiles are assumed to mean that the weight percent value for a species is zero and is included in determining the median value for the composite profile. OC and EC composite values are calculated by the following method to account for differing analytical methods:

1. Prior to profile compositing, the OC and EC fractions are summed to calculate TC for each source profile.

2. The mean OC, mean EC, and mean TC values are calculated for each source category. If any SPECIATE profiles in a source category measured carbon using a TOR method, then only those profiles are included in the mean calculations. If no profiles in the category measured carbon by TOR, then all profiles are used to calculate mean OC, EC, and TC values.

3. Two ratios are calculated using the above mean values for each source category: OC:TC and EC:TC.

4. "Carbon method corrected" OC and EC values are calculated for each SPECIATE profile by multiplying the source category specific OC:TC and EC:TC ratios against the original TC values of each source profile.

5. The medians of these "Carbon method corrected" OC and EC values in each source category are taken as the final value for the composite profile of each source category.

In addition to PM composite profiles, there are a set of composite TOG profiles (95325 – 95333, 95398 – 95408, 95417 – 95428) added to SPECIATE 4.5. Profiles 95325 (Chemical manufacturing industry wide composite) and 95326 (Pulp and paper industry wide composite) are composites based on the median of each species and re-normalized by the sum of species (EPA Work Assignment WA 2-02). Profiles 95398 and 95399 – 95408 are a set of composite profiles representing oil and natural gas production industry in Colorado and California, respectively. These oil and natural gas production industry composites are based on the mean of individual profiles in the same emission source type (e.g., oil well tanks), because some of them only have two to five individual profiles and no meaningful median composites can be calculated. For the case of Profile

95398, it was found that the compositions are very comparable when they are based on median and mean. This is because the sample size (27 individual profiles) is relatively large and their compositions are similar.

Composite TOG profile numbers 95417 – 95420 are based on individual TOG profiles reported by oil production companies in the EPA Region 8 Tribal Minor Source Registration database. Individual profiles of the same source type (e.g., oil tank battery vent gas) are weighted by respective company oil or natural gas production rate to calculate the composite profile (e.g., Profile 95419) to represent the "Oil Field - Condensate Tank Battery Vent Gas" in Uinta Basin, Utah.

Profiles 95421 – 95428 are composite TOG profiles based on reviews of the current state of knowledge regarding the chemical composition of emissions and emission factors for prescribed burning and wildfires in United States (Urbanski, 2014).

N. Molecular Weights

The SPECIATE 4.5 database contains a SPECIE_PROPERTIES table that includes 2,602 unique species (both individual compounds and mixtures). Since SPECIATE 4.5 includes all profiles from SPECIATE 3.2, the molecular weights (MWs) as well as other species information are included in the SPECIATE 4.5 database. The MWs for new species are obtained from the EPA's SRS database. If the MW for a species is not available in the SRS, then internet search engines are utilized to look for a MW. Alternatively, the molecular weight from the same class of compounds is applied. For example, Species ID 2624 (1,4-Dimethyl-2-ethylcyclohexane), the molecular weight of 1,3-Dimethyl-2-ethylcyclohexane is used. If a MW cannot be identified for a species, a default average MW (i.e., 137.19 grams/mole) is assumed. This default MW is recommended by Dr. William Carter of University of California at Riverside who uses the value to process input files for air quality modeling.

O. Quality Assurance Project Plan

A "SPECIATE 4.0 Quality Management Plan/Quality Assurance Project Plan" was developed at the beginning of the SPECIATE update project, and has been updated for SPECIATE 4.4 to document changes in quality assurance/quality control responsibilities and refinements to procedures. The updated QAPP was used as is for SPECIATE 4.5. This document is available on EPA's SPECIATE webpage.

P. Protocol for Revising Speciation Profiles in a Published Version of the SPECIATE Database

A new and important part of the SPECIATE project is how to revise the database if a profile becomes outdated or an error is discovered in a profile's underlying data. As the Workgroup continues to add new source profiles and improve the functions and quality of the database, the Workgroup has identified source profiles with incorrect weight percent and/or compound entries. For example, there have been errors discovered in the laboratory reported data that were used for SPECIATE. Since some of those problematic profiles were used in past modeling and/or emission inventory assessments, the Workgroup recommends not changing or removing any numbers from previously published SPECIATE versions. The Workgroup's reason is that the numbers, regardless of accuracy, have been used in modeling and elsewhere and it would be impossible to change all of the published literature and unpublished decisions. The consensus recommendation is that a notation should be included in the database where profiles have changed subsequent to their original publication in SPECIATE.

Below are the changes and notes that are made to the SPECIATE database, once it is confirmed with the data sources that a profile(s) is incorrect.

1. A note indicating the errors and replacing profile numbers is added in the NOTES field in the GAS_PROFILE or PM_PROFILE tables;
2. The note is then documented in the REVISION_LIST table that records all changes made to the database. (Since this table is not part of SPECIATE database, it is posted on SharePoint for internal use only by the Workgroup. It is also available from the EPA work assignment manager Mike Kosusko); and
3. The corrected profile is added to the database and assigned the original profile number, e.g., profile number 4567, with an alpha notation like 4567a and further refinements with b, c, d, and so on.

CHAPTER V. Source Profile Preparation Methods

Chemical speciation data of air pollution sources are typically provided in one of three common formats – weight percent format, emission factor format, or weight percent of carbon. The methods used to prepare speciation profiles for SPECIATE depend upon the format of the speciated data as described below:

- *Weight percent format* – both CARB and DRI speciated datasets are provided in weight percent format, which only need to be augmented with profile metadata to support the new SPECIATE tables described above (i.e., keywords, documentation, analytical and sampling methods, profile quality ratings, pollution source descriptions, etc.). EPA gasoline and diesel profiles are also available in weight percent format, and therefore undergo the same processing procedures as CARB and DRI profiles, except that oxygenates (ethanol, MTBE, and TAME) are adjusted based on response factors by GC/FID (Lewis, 2004) as described in subsection H. After applying corrections, the fuels profiles are normalized to 100%.

- *Emission factor format* – EPA foliar fuels speciation data and speciation data from the California Institute of Technology are available as emission factors (e.g., mg/kilogram of biomass burned, mg/kilometer traveled, and mg/kilogram of meat cooked). For each source type, emission factors of all speciated compounds and unidentified species (when available) are summed to obtain the total VOC or TOG emission factors. The individual species emission factors are then divided by the total emission factors and multiplied by 100 to convert to weight percent. The normalization bases of VOC or TOG can sometimes be measured with instruments and analytical methods that are different from those used to determine speciation. For cases when the reported VOC or TOG normalization bases are larger than the sum of speciated mass, the remaining unidentified species mass (called "Unknown") is added to the profile to generate the total VOC or TOG. Part of the discrepancy is due to the fact that different analytical methods applied in each speciation sample are more accurate for certain sets of compounds than others. Also note that, since the unidentified species are unknown, their masses are often not quantifiable. The unidentified compounds are usually unresolved mixtures with GC.

- *Weight percent of carbon format* – few speciation data sets are reported in weight percent of carbon, instead of the entire molecule. Using ethane (C_2H_6) as an example, the mass from the two carbons was reported, but not for hydrogen atoms. The carbon mass is converted to account for the whole molecule mass by [Wt. C% × ethane molecular weight (30.07)] ÷ [2 × carbon molecular weight (12.01)]. After converting all compounds, the entire profile is normalized by the sum of converted weight percent.

In some instances, organic compounds in PM are also speciated. These organic species are divided by PM mass, as is done for other ions and elements in PM. For PM profiles, PM-associated organic species mass is not included in the PM mass to avoid double-counting with OC (i.e., carbon atoms in each organic species are already represented in the OC fraction). After obtaining the weight fraction for each species, this value is multiplied by 100 to obtain weight percent.

After converting speciated data to weight percent, the profile information listed in the data dictionary (e.g., CAS number, keywords, documentation, analytical and sampling methods, profile quality ratings, pollution source descriptions) is added based on the information provided in the original reference(s) for each profile (e.g., peer-reviewed papers and technical reports).

Many organic species have several chemical names (e.g., methylene chloride and dichloromethane). The database has been revised to be consistent with the nomenclature used commonly within the United States (e.g., from sources such as chemfinder.com). These chemical names are consistent with those available in the EPA Substance Registry Services (SRS) database (https://iaspub.epa.gov/sor_internet/registry/substreg/searchandretrieve/substancesearch/search.do). In addition, errors have been found for some of the CAS numbers provided in the original speciation data. Therefore, CAS numbers are checked by a program following the design of the CAS numbering system (CAS, 2004).

Limitations of SPECIATE 4.5 include the following:

1. "Unknown," "Unidentified," and "Undefined VOC" species – In SPECIATE 4.1 and earlier versions (i.e., 3.2 and 4.0), several profiles contain unspeciated mass identified as "Unknown," "Unidentified," or "Undefined VOC". In some cases, more than one of these terms appears in the same profile. Users should know that all three terms represent the mass associated with unidentified species in the profile. For SPECIATE 4.2 and later versions of SPECIATE, the Workgroup decided to use one term, "Unknown," to identify unspeciated mass in profiles. The database has been revised accordingly.

2. Use of profiles with low quality ratings – Profile quality ratings are dictated by the age or vintage of the data (V-rating) and number of samples (D-rating). For example, Profiles #4526 – 4534 are gasoline vapor profiles collected in 2004. Even though, these profiles are relatively recent and provide comprehensive coverage of species, they have an overall quality rating of "E" because they are based on one sample. Note that gasoline fuels of different grades and produced by different refineries can have a wide range of gasoline vapor compositions. For example, in the same set of profiles (#4526 – 4534), n-butane varies from 22% to 41%. Therefore, the species composition of the individual profiles can vary significantly even though samples were collected from the same area in the same month. In this case, a composite profile based on those profiles (#4526 – 4534) is recommended. Low quality rating profiles should be used with caution since the low rating often indicates source sectors for which profiles are based on a single sample.

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APPENDIX A. Listing of New Profiles Added to the SPECIATE 4.5 Database

See Table A-1 on next page.

Table A-1. List of New Organic Gas Profiles Added to the SPECIATE 4.5 Database

Profile Number	Name	Profile Type	Keyword
95077	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95078	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95079	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95080	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95081	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95082	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95083	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95084	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95085	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95086	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95087	Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95087a	Composite - Oil Field - Oil Tank Battery Vent Gas	G	Oil Field; Oil Tank Battery Vent Gas
95088	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95089	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95090	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95091	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95092	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95093	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95094	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95095	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95096	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95097	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95098	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95099	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95100	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95101	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas

Profile Number	Name	Profile Type	Keyword
95102	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95103	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95104	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95105	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95106	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95107	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95108	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95109	Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95109a	Composite - Oil Field - Condensate Tank Battery Vent Gas	G	Oil Field; Condensate Tank Battery Vent Gas
95111	Gasoline Exhaust - Tunnel Study	G	Gasoline Exhaust; Tunnel Study
95112	Unburned Gasoline Exhaust - Tunnel Study	G	Unburned Gasoline Exhaust; Tunnel Study
95113	Diesel Exhaust - Tunnel Study	G	Diesel Exhaust; Tunnel Study
95114	Unburned Diesel Exhaust - Tunnel Study	G	Unburned Diesel Exhaust; Tunnel Study
95115	Gasoline - California composite	G	Gasoline
95116	Gasoline - Bakersfield	G	Gasoline
95117	Gasoline - Berkeley	G	Gasoline
95118	Gasoline - Pasadena	G	Gasoline
95119	Gasoline - Sacramento	G	Gasoline
95120	Diesel - California composite	G	Diesel
95121	Diesel - Bakersfield	G	Diesel
95122	Diesel - Berkeley	G	Diesel
95123	Diesel - Pasadena	G	Diesel
95124	Diesel - Sacramento	G	Diesel
95129	Residential Wood Combustion - Pellet Stove	G	Pellet Stove; Residential Wood Combustion
95130	Residential Wood Combustion - Pellet Stove	G	Pellet Stove; Residential Wood Combustion
95131	Residential Wood Combustion - Pellet Stove	G	Pellet Stove; Residential Wood Combustion
95132	Residential Wood Combustion - Pellet Stove	G	Pellet Stove; Residential Wood Combustion
95133	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion

Profile Number	Name	Profile Type	Keyword
95134	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion
95135	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion
95136	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion
95137	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion
95138	Residential Wood Combustion - Wood Stove	G	Wood Stove; Residential Wood Combustion
95156	Residential Wood Combustion - Wood Stove - Maple	G	Wood Stove; Residential Wood Combustion; Maple
95157	Residential Wood Combustion - Wood Stove - Spruce	G	Wood Stove; Residential Wood Combustion; Spruce
95158	Residential Wood Combustion - Wood Stove - Maple	G	Wood Stove; Residential Wood Combustion; Maple
95159	Residential Wood Combustion - Wood Stove - Spruce	G	Wood Stove; Residential Wood Combustion; Spruce
95160	Prescribed Burning - Flaming Stage	G	Prescribed Burning; Flaming Stage
95161	Prescribed Burning - Smoldering Stage	G	Prescribed Burning; Smoldering Stage
95211	Oil and Gas Extraction Field	G	Oil and Gas Extraction Field
95212	Vehicle Exhaust - Tunnel Study - Fleet Speed 45 km/hr	G	Vehicle Exhaust; Tunnel Study; Fleet Speed 45 km/hr
95213	Vehicle Exhaust - Tunnel Study - Fleet Speed 65 km/hr	G	Vehicle Exhaust; Tunnel Study; Fleet Speed 65 km/hr
95214	Vehicle Exhaust - Tunnel Study - Fleet Speed 75 km/hr	G	Vehicle Exhaust; Tunnel Study; Fleet Speed 75 km/hr
95215	Vehicle Exhaust - Tunnel Study - Fleet Speed 85 km/hr	G	Vehicle Exhaust; Tunnel Study; Fleet Speed 85 km/hr
95216	Vehicle Exhaust - Tunnel Study - Gasoline - Diesel - LGP	G	Vehicle Exhaust; Tunnel Study; Gasoline-Diesel-LPG Vehicles
95217	Vehicle Exhaust - Tunnel Study - Gasoline and Diesel Vehicles	G	Vehicle Exhaust; Tunnel Study; Gasoline and Diesel Vehicles
95218	Vehicle Exhaust - Tunnel Study - Gasoline and Diesel Vehicles	G	Vehicle Exhaust; Tunnel Study; Gasoline and Diesel Vehicles
95221	Petroleum operations - extraction, processing, transmission	G	Petroleum Operations
95222	Poultry Production - Empty Building	G	Poultry Production
95223	Poultry Production - Average of Production Cycle	G	Poultry Production
95224	Poultry Production - Production Cycle	G	Poultry Production
95225	Poultry Production - Production Cycle	G	Poultry Production
95226	Poultry Production - Production Cycle	G	Poultry Production
95227	Heavy Duty Diesel Exhaust - Euro3	G	Heavy Duty Diesel Exhaust; Euro3
95228	Heavy Diesel Exhaust - biodiesel fuels - Euro3	G	Heavy Diesel Exhaust; biodiesel fuels; Euro3
95229	Light Duty Diesel Exhaust - diesel and biodiesel - Euro4	G	Light Duty Diesel Exhaust; diesel and biodiesel; Euro4

Profile Number	Name	Profile Type	Keyword
95230	Light Duty Gasoline Exhaust - Euro3	G	Light Duty Gasoline Exhaust; Euro3
95231	Moped - 2-stroke - PreEuro	G	Moped; 2-stroke; PreEuro
95232	Moped - 2-stroke - Euro1	G	Moped; 2-stroke; Euro1
95233	Moped - 2-stroke - Euro1	G	Moped; 2-stroke; Euro1
95234	Moped - 2-stroke - Euro1 - LPG	G	Moped; 2-stroke; Euro1; LPG
95235	Moped - 2-stroke - Euro2	G	Moped; 2-stroke; Euro2
95236	Moped - 2-stroke - Euro2	G	Moped; 2-stroke; Euro2
95237	Moped - 2-stroke - Euro2	G	Moped; 2-stroke; Euro2
95238	Light Duty Gasoline Exhaust - Euro4 - FLEX Car - E0 and E10 gasoline	G	Light Duty Gasoline Exhaust; Euro4; FLEX Car; E0 and E10 gasoline
95239	Light Duty Gasoline Exhaust - Euro4 - FLEX Car - E85 gasoline	G	Light Duty Gasoline Exhaust; Euro4; FLEX Car; E85 gasoline
95240	Beef Cattle Farm and Animal Waste	G	Beef Cattle Farm; Animal Waste
95241	Swine Farm and Animal Waste	G	Swine Farm; Animal Waste
95242	Poultry Farm - Hen and Animal Waste	G	Poultry Farm; Animal Waste
95243	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95244	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95245	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95246	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95247	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95248	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95249	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95250	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95251	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95252	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95253	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95254	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95255	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95256	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95257	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well

Profile Number	Name	Profile Type	Keyword
95258	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95259	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95260	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95261	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95262	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95263	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95264	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95265	Natural Gas - Untreated - Tank Battery of Oil Well	G	Natural Gas; Tank Battery of Oil Well
95266	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95267	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95268	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95269	Natural Gas - Untreated - Tank for Several Oil Wells	G	Natural Gas; Tank for Several Oil Wells
95270	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95271	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95272	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95273	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95274	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95275	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95276	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95277	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95278	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95279	Natural Gas - Untreated - Well Casing of Oil Well	G	Natural Gas; Well Casing of Oil Well
95280	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95281	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95282	Natural Gas - Untreated - Well Casing of Oil Well	G	Natural Gas; Well Casing of Oil Well
95283	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95284	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95285	Natural Gas - Untreated - Gas Well with Condensate	G	Natural Gas; Gas Well with Condensate

Profile Number	Name	Profile Type	Keyword
95286	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95287	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95288	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95289	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95290	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95291	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95292	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95293	Natural Gas - Untreated - Tank for Several Oil Wells	G	Natural Gas; Tank for Several Oil Wells
95294	Natural Gas - Untreated - Oil and Gas Separator	G	Natural Gas; Oil and Gas Separator
95295	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95296	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95297	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95298	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95299	Natural Gas - Untreated - Oil and Condensate Well	G	Natural Gas; Oil and Condensate Well
95300	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95301	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95302	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95303	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95304	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95305	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95306	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95307	Natural Gas - Untreated - Gas and Condensate Well	G	Natural Gas; Gas and Condensate Well
95308	Natural Gas - Untreated - Oil Well Separator	G	Natural Gas; Oil Well Separator
95309	Natural Gas - Untreated - Gas Well Separator	G	Natural Gas; Gas Well Separator
95310	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95311	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95312	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95313	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well

Profile Number	Name	Profile Type	Keyword
95314	Natural Gas - Untreated - Oil Well Separator	G	Natural Gas; Oil Well Separator
95315	Natural Gas - Untreated - Gas Well	G	Natural Gas; Gas Well
95316	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95317	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95318	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95319	Natural Gas - Untreated - Oil Well	G	Natural Gas; Oil Well
95320	Light Duty Diesel Exhaust - Phase 1	G	Light Duty Diesel Exhaust; Phase 1
95321	Light Duty Diesel Exhaust - Phase 2	G	Light Duty Diesel Exhaust; Phase 2
95322	Light Duty Diesel Exhaust - Phase 3	G	Light Duty Diesel Exhaust; Phase 3
95323	Light Duty Diesel Exhaust - FTP-75 Cycle	G	Light Duty Diesel Exhaust; FTP-75 Cycle
95324	Light Duty Diesel Exhaust - Highway Fuel Economy Cycle	G	Light Duty Diesel Exhaust; Highway Fuel Economy Cycle
95325	Chemical Manufacturing Industry Wide Composite	G	Composite Profile; Chemical Manufacturing
95326	Pulp and Paper Industry Wide Composite	G	Composite Profile; Pulp and Paper Mills
95327	Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - Non-oxygenated gasoline	G	Spark-Ignition Exhaust; 2-stroke off-road engines; Non-oxygenated gasoline; All terrain vehicle; Nonroad motorcycle
95328	Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - E10 ethanol gasoline	G	Spark-Ignition Exhaust; 2-stroke off-road engines; E10 ethanol gasoline; All terrain vehicle; Nonroad motorcycle
95329	Spark-Ignition Exhaust Emissions from 4-stroke off-road engines - Non-oxygenated gasoline	G	Spark-Ignition Exhaust; 4-stroke off-road engines; Non-oxygenated gasoline; Lawn and garden engines
95330	Spark-Ignition Exhaust Emissions from 4-stroke off-road engines - E10 ethanol gasoline	G	Spark-Ignition Exhaust; 4-stroke off-road engines; E10 ethanol gasoline; Lawn and garden engines
95331	Diesel Exhaust Emissions from Pre-Tier 1 Off-road Engines	G	Diesel Exhaust Emissions; Pre-Tier 1 Off-road Engines
95332	Diesel Exhaust Emissions from Tier 1 Off-road Engines	G	Diesel Exhaust Emissions; Tier 1 Off-road Engines
95333	Diesel Exhaust Emissions from Tier 2 Off-road Engines	G	Diesel Exhaust Emissions; Tier 2 Off-road Engines
95335	Diesel Exhaust - Heavy-heavy duty truck - 2011 model year	G	Diesel Exhaust; Heavy-heavy duty truck; 2011 model year; Ultra-low sulfur diesel
95336	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 1	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95337	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 2	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95338	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 3	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95339	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 5	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95340	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 6	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin

Profile Number	Name	Profile Type	Keyword
95341	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 9	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95342	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 10	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95343	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 11	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95344	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 12	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95345	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 13	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95346	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 14	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95347	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 15	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95348	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 16	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95349	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 17	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95350	Oil and Gas Production - Untreated Natural Gas, Uinta Basin–Operator 18	G	Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95351	Oil and Gas Production - Oil Tank Vent Gas, Uinta Basin–Operator 1	G	Oil and Gas Production; Oil Tank Vent Gas; Uinta Basin
95352	Oil and Gas Production - Oil Tank Vent Gas, Uinta Basin–Operator 2	G	Oil and Gas Production; Oil Tank Vent Gas; Uinta Basin
95353	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 4	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95354	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 5	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95355	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 6	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95356	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 7	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95357	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 8	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95358	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 9	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95359	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 11	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95360	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 12	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95361	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 14	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95362	Oil and Gas Production - Oil Tank Vent Gas, Uinta Basin–Operator 15	G	Oil and Gas Production; Oil Tank Vent Gas; Uinta Basin
95363	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 17	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95364	Oil and Gas Production - Condensate Tank Vent Gas, Uinta Basin–Operator 18	G	Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95365	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95366	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank

Profile Number	Name	Profile Type	Keyword
95368	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95370	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95371	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95372	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95373	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95374	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95375	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95377	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95379	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95380	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95381	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95383	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95384	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95385	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95386	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95387	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95388	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95389	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95390	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95391	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95392	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95394	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95395	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95396	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95397	Oil and Natural Gas Production - Condensate Tank	G	Oil and Natural Gas Production; Condensate Tank
95398	Composite Profile - Oil and Natural Gas Production - Condensate Tanks	G	Composite Profile; Oil and Natural Gas Production; Condensate Tank
95399	Composite Profile - Oil Field - Wells	G	Composite Profile; Oil Wells
95400	Composite Profile - Oil Field - Tanks	G	Composite Profile; Oil Well Tanks

Profile Number	Name	Profile Type	Keyword
95401	Composite Profile - Oil Field - Separators	G	Composite Profile; Oil Field; Separators
95402	Composite Profile - Oil Field - Vapor Recovery	G	Composite Profile; Oil Field; Vapor Recovery
95403	Composite Profile - Gas Wells	G	Composite Profile; Gas Wells
95404	Composite Profile - Oil Wells	G	Composite Profile; Oil Wells
95405	Composite Profile - Oil and Gas Separators	G	Composite Profile; Oil and Gas Separators
95406	Composite Profile - Oil Well Tanks	G	Composite Profile; Oil Well Tanks
95407	Composite Profile - Oil Well Casings	G	Composite Profile; Oil Well Casings
95408	Composite Profile - Gas and Oil Condensate Wells	G	Composite Profile; Gas and Oil Condensate Wells
95409	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 6	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95410	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 9	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95411	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 10	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95412	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 11	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95413	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 12	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95414	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 15	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95415	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 17	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95416	Oil and Gas Production - Glycol Dehydrator, Uinta Basin–Operator 18	G	Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95417	Oil and Gas Production - Composite Profile - Untreated Natural Gas, Uinta Basin	G	Composite Profile; Natural Gas; Untreated; Raw Gas; Oil and Gas Production; fugitive leaks, pneumatic controllers; pneumatic pumps; Uinta Basin
95418	Oil and Gas Production - Composite Profile - Condensate Tank Vent Gas, Uinta Basin	G	Composite Profile; Oil and Gas Production; Condensate Tank Vent Gas; Uinta Basin
95419	Oil and Gas Production - Composite Profile - Oil Tank Vent Gas, Uinta Basin	G	Composite Profile; Oil and Gas Production; Oil Tank Vent Gas; Uinta Basin
95420	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Uinta Basin	G	Composite Profile; Oil and Gas Production; Glycol Dehydrator; Uinta Basin
95421	Composite Profile - Prescribed fire southeast conifer forest	G	Composite Profile; Prescribed fire southeast conifer forest
95422	Composite Profile - Prescribed fire southwest conifer forest	G	Composite Profile; Prescribed fire southwest conifer forest
95423	Composite Profile - Prescribed fire northwest conifer forest	G	Composite Profile; Prescribed fire northwest conifer forest
95424	Composite Profile - Wildfire northwest conifer forest	G	Composite Profile; Wildfire northwest conifer forest
95425	Composite Profile - Wildfire boreal forest	G	Composite Profile; Wildfire boreal forest
95426	Composite Profile - Residual smoldering combustion - Stumps and Logs	G	Composite Profile; Residual smoldering combustion; Stumps and Logs
95427	Composite Profile - Residual smoldering combustion - Temperate forest duff/organic soil	G	Composite Profile; Residual smoldering combustion; Temperate forest duff/organic soil
95428	Composite Profile - Residual smoldering combustion - Boreal forest duff/organic soil	G	Composite Profile; Residual smoldering combustion; Boreal forest duff/organic soil

Profile Number	Name	Profile Type	Keyword
DJFLA_R	Oil and Gas -Denver-Julesburg Basin Flashing Gas Composition for Condensate Tanks	G	Flash gas for condensate tank
DJVNT_R	Oil and Gas -Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	G	Produced Gas
FLR70	Natural Gas Flare Profile with DRE <80%	G	Natural Gas Flare
FLR88	Natural Gas Flare Profile with DRE >80-95%	G	Natural Gas Flare
FLR97	Natural Gas Flare Profile with DRE >95-98%	G	Natural Gas Flare
FLR99	Natural Gas Flare Profile with DRE >98%	G	Natural Gas Flare
PNC01_R	Oil and Gas -Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	G	Produced Gas
PNC02_R	Oil and Gas -Piceance Basin Produced Gas Composition from Oil Wells	G	Produced Gas; Oil Wells
PNC03_R	Oil and Gas -Piceance Basin Flash Gas Composition for Condensate Tank	G	Flash gas for condensate tank
PNCDH	Oil and Gas Production - Composite Profile - Glycol Dehydrator, Piceance Basin	G	Oil and Gas Production; Glycol Dehydrator; Piceance Basin
PRBCB_R	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	G	Coalbed Methane (CBM); Produced Gas
PRBCO_R	Oil and Gas -Powder River Basin Produced Gas Composition from Non-CBM Wells	G	Produced Gas
PRM01_R	Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells	G	Produced Gas
SSJCB_R	Oil and Gas -South San Juan Basin Produced Gas Composition from CBM Wells	G	Coalbed Methane (CBM); Produced Gas
SSJCO_R	Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	G	Produced Gas
SWFLA_R	Oil and Gas -SW Wyoming Basin Flash Gas Composition for Condensate Tanks	G	Flash gas for condensate tank
SWVNT_R	Oil and Gas -SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	G	Produced Gas
UNT01_R	Oil and Gas -Uinta Basin Produced Gas Composition from CBM Wells	G	Coalbed Methane (CBM); Produced Gas
UNT02_R	Oil and Gas -Uinta Basin Produced Gas Composition from Non-CBM Wells	G	Produced Gas
UNT03_R	Oil and Gas -Uinta Basin Flash Gas Composition from Oil Tanks	G	Flash gas for oil tank
UNT04_R	Oil and Gas -Uinta Basin Flash Gas Composition from Condensate Tanks	G	Flash gas for condensate tank
WRBCO_ R	Oil and Gas -Wind River Basin Produced Gas Composition from Non-CBM Gas Wells	G	Produced Gas

Table A-2. Summary of New PM Profiles Added to the SPECIATE 4.5 Database

Profile Number	Name	Profile Type	Keyword
95000	Indoor Open Wood Cooking Fire	P	Indoor Open Wood Cooking Fire
95001	Indoor Open Wood Cooking Fire	P	Indoor Open Wood Cooking Fire
95002	Indoor Open Wood Cooking Fire	P	Indoor Open Wood Cooking Fire
95003	Indoor Open Wood Cooking Fire	P	Indoor Open Wood Cooking Fire
95004	Indoor Open Wood Cooking Fire	P	Indoor Open Wood Cooking Fire
95005	Garbage Burning	P	Garbage Burning
95006	Garbage Burning	P	Garbage Burning
95007	Garbage Burning	P	Garbage Burning
95008	Brick Making Kiln	P	Brick Making Kiln
95009	Brick Making Kiln	P	Brick Making Kiln
95010	Charcoal Making Kiln	P	Charcoal Making Kiln
95011	Charcoal Making Kiln	P	Charcoal Making Kiln
95012	Barley Stubble Field Burning	P	Barley Stubble Field Burning
95013	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (-7 oC)
95014	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E0 gasoline; (-7 oC)
95015	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E0 gasoline; (-7 oC)
95016	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (-7 oC)
95017	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (-7 oC)
95018	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (-7 oC)
95019	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (-7 oC)
95020	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (-7 oC)
95021	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E85 gasoline; (-7 oC)
95022	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E85 gasoline; (-7 oC)
95023	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E85 gasoline; (-7 oC)
95024	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E85 gasoline; (-7 oC)

Profile Number	Name	Profile Type	Keyword
95025	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (24 oC)
95026	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E0 gasoline; (24 oC)
95027	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E0 gasoline; (24 oC)
95028	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (24 oC)
95029	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (24 oC)
95030	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (24 oC)
95031	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (24 oC)
95032	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (24 oC)
95033	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E85 gasoline; (24 oC)
95034	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E85 gasoline; (24 oC)
95035	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E85 gasoline; (24 oC)
95036	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E85 gasoline; (24 oC)
95037	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (-7 oC)
95038	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E0 gasoline; (-7 oC)
95039	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E0 gasoline; (-7 oC)
95040	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (-7 oC)
95041	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (-7 oC)
95042	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (-7 oC)
95043	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (-7 oC)
95044	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (-7 oC)
95045	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E85 gasoline; (-7 oC)
95046	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E85 gasoline; (-7 oC)
95047	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E85 gasoline; (-7 oC)
95048	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E85 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E85 gasoline; (-7 oC)
95049	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (24 oC)
95050	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E0 gasoline; (24 oC)
95051	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E0 gasoline; (24 oC)

Profile Number	Name	Profile Type	Keyword
95052	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (24 oC)
95053	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (24 oC)
95054	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (24 oC)
95055	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (24 oC)
95056	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (24 oC)
95057	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E85 gasoline; (24 oC)
95058	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E85 gasoline; (24 oC)
95059	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E85 gasoline; (24 oC)
95060	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E85 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E85 gasoline; (24 oC)
95061	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (-7 oC)
95062	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E0 gasoline; (-7 oC)
95063	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E0 gasoline; (-7 oC)
95064	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (-7 oC)
95065	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (-7 oC)
95066	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (-7 oC)
95067	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (-7 oC)
95068	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (-7 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (-7 oC)
95069	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E0 gasoline; (24 oC)
95072	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E0 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E0 gasoline; (24 oC)
95073	Gasoline Exhaust SVOC - LA92 UDC cycle cold start (phase 1) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; cold start (phase 1); E10 gasoline; (24 oC)
95074	Gasoline Exhaust SVOC - LA92 UDC cycle hot-stabilized phase (phase 2) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; hot-stabilized phase (phase 2); E10 gasoline; (24 oC)
95075	Gasoline Exhaust SVOC - LA92 UDC cycle warm-start transient phase combined with hot-stabilized phase (phase 34) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; warm-start transient phase combined with hot-stabilized phase (phase 34); E10 gasoline; (24 oC)
95076	Gasoline Exhaust SVOC - LA92 UDC cycle (phase 1234) - E10 gasoline - (24 oC)	P	Gasoline Exhaust SVOC; LA92 UDC cycle; phase 1234; E10 gasoline; (24 oC)
95125	Gas-fired boiler exhaust	P	Gas-fired boiler exhaust
95126	Gas-fired process heater exhaust	P	Gas-fired process heater exhaust
95127	Gas-fired internal combustion combined cycle/cogeneration plant exhaust	P	Gas-fired internal combustion combined cycle/cogeneration plant exhaust
95128	Institutional boiler exhaust fueled with No. 6 oil	P	Institutional boiler exhaust fueled with No. 6 oil

Profile Number	Name	Profile Type	Keyword
95139	Sewage Sludge Incineration	P	Sewage Sludge Incineration
95140	Sewage Sludge Incineration	P	Sewage Sludge Incineration
95141	Sewage Sludge Incineration	P	Sewage Sludge Incineration
95142	Sewage Sludge Incineration	P	Sewage Sludge Incineration
95143	Municipal Sewage Sludge	P	Sewage Sludge
95144	Municipal Sewage Sludge	P	Sewage Sludge
95145	Municipal Sewage Sludge	P	Sewage Sludge
95146	Municipal Sewage Sludge	P	Sewage Sludge
95147	Biomass Burning - ponderosa pine wood	P	Biomass Burning; ponderosa pine wood
95148	Biomass Burning - ponderosa pine needles	P	Biomass Burning; ponderosa pine needles
95149	Biomass Burning - white pine needles	P	Biomass Burning; white pine needles
95150	Biomass Burning - sagebrush	P	Biomass Burning; sagebrush
95151	Biomass Burning - excelsior	P	Biomass Burning; excelsior
95152	Biomass Burning - Dambo grass	P	Biomass Burning; Dambo grass
95153	Biomass Burning - Montana grass	P	Biomass Burning; Montana grass
95154	Biomass Burning - tundra core	P	Biomass Burning; tundra core
95155	Kerosene combustion soot	P	Kerosene combustion soot
95162	Prescribed Burning	P	Prescribed Burning
95163	Coal Combustion - Fluidized-Bed Incinerator	P	Coal Combustion; Fluidized-Bed Incinerator
95164	Coal Combustion - Fluidized-Bed Incinerator	P	Coal Combustion; Fluidized-Bed Incinerator
95165	Coal Combustion - Fluidized-Bed Incinerator	P	Coal Combustion; Fluidized-Bed Incinerator
95166	Welding Fume - High Heat - UONI 13/45 Electrode	P	Welding Fume
95167	Welding Fume - High Heat - UONI 13/45 Electrode	P	Welding Fume
95168	Welding Fume - High Heat - UONI 13/45 Electrode	P	Welding Fume
95169	Welding Fume - Low Heat - UONI 13/45 Electrode	P	Welding Fume
95170	Welding Fume - High Heat - ANO-4 Electrode	P	Welding Fume
95171	Welding Fume - High Heat - ANO-4 Electrode	P	Welding Fume
95172	Welding Fume - High Heat - ANO-4 Electrode	P	Welding Fume

Profile Number	Name	Profile Type	Keyword
95173	Welding Fume - Low Heat - ANO-4 Electrode	P	Welding Fume
95174	Welding Fume - High Heat - ANO-4i Electrode	P	Welding Fume
95175	Welding Fume - High Heat - ANO-4i Electrode	P	Welding Fume
95176	Welding Fume - High Heat - ANO-4i Electrode	P	Welding Fume
95177	Welding Fume - Low Heat - ANO-4i Electrode	P	Welding Fume
95178	Coal Combustion - Fly Ash - Anthracite Coal	P	Coal Combustion; Fly Ash; Anthracite Coal; Heating Facility
95179	Coal Combustion - Fly Ash - Anthracite Coal	P	Coal Combustion; Fly Ash; Anthracite Coal; Heating Facility
95180	Coal Combustion - Fly Ash - Anthracite Coal	P	Coal Combustion; Fly Ash; Anthracite Coal; Heating Facility
95181	Coal Combustion - Fly Ash - Anthracite Coal	P	Coal Combustion; Fly Ash; Anthracite Coal; Home Heating
95182	Residential Wood Stove Combustion - White Oak	P	Residential Wood Stove Combustion; White Oak
95183	Residential Wood Stove Combustion - White Oak	P	Residential Wood Stove Combustion; White Oak
95184	Residential Wood Stove Combustion - Red Maple	P	Residential Wood Stove Combustion; Red Maple
95185	Residential Wood Stove Combustion - Sugar Maple	P	Residential Wood Stove Combustion; Sugar Maple
95186	Residential Wood Stove Combustion - Douglas Fir	P	Residential Wood Stove Combustion; Douglas Fir
95187	Residential Wood Stove Combustion - Douglas Fir	P	Residential Wood Stove Combustion; Douglas Fir
95188	Residential Wood Stove Combustion - Loblolly Pine	P	Residential Wood Stove Combustion; Loblolly Pine
95189	Fireplace Wood Combustion - White Oak	P	Fireplace Wood Combustion; White Oak
95190	Fireplace Wood Combustion - Sugar Maple	P	Fireplace Wood Combustion; Sugar Maple
95191	Fireplace Wood Combustion - Black Oak	P	Fireplace Wood Combustion; Black Oak
95192	Fireplace Wood Combustion - American Beech	P	Fireplace Wood Combustion; American Beech
95193	Fireplace Wood Combustion - Black Cherry	P	Fireplace Wood Combustion; Black Cherry
95194	Fireplace Wood Combustion - Quaking Aspen	P	Fireplace Wood Combustion; Quaking Aspen
95195	Fireplace Wood Combustion - White Spruce	P	Fireplace Wood Combustion; White Spruce
95196	Fireplace Wood Combustion - Douglas Fir	P	Fireplace Wood Combustion; Douglas Fir
95197	Fireplace Wood Combustion - Ponderosa Pine	P	Fireplace Wood Combustion; Ponderosa Pine
95198	Fireplace Wood Combustion - Pinyon Pine	P	Fireplace Wood Combustion; Pinyon Pine
95199	Fireplace Wood Combustion - Red Maple	P	Fireplace Wood Combustion; Red Maple
95200	Fireplace Wood Combustion - Northern Red Oak	P	Fireplace Wood Combustion; Northern Red Oak

Profile Number	Name	Profile Type	Keyword
95201	Fireplace Wood Combustion - Paper Birch	P	Fireplace Wood Combustion; Paper Birch
95202	Fireplace Wood Combustion - Eastern White Pine	P	Fireplace Wood Combustion; Eastern White Pine
95203	Fireplace Wood Combustion - Eastern Hemlock	P	Fireplace Wood Combustion; Eastern Hemlock
95204	Fireplace Wood Combustion - Balsam Fir	P	Fireplace Wood Combustion; Balsam Fir
95205	Fireplace Wood Combustion - Yellow Poplar	P	Fireplace Wood Combustion; Yellow Poplar
95206	Fireplace Wood Combustion - White Ash	P	Fireplace Wood Combustion; White Ash
95207	Fireplace Wood Combustion - Sweetgum	P	Fireplace Wood Combustion; Sweetgum
95208	Fireplace Wood Combustion - Mockernut Hickory	P	Fireplace Wood Combustion; Mockernut Hickory
95209	Fireplace Wood Combustion - Loblolly Pine	P	Fireplace Wood Combustion; Loblolly Pine
95210	Fireplace Wood Combustion - Slash Pine	P	Fireplace Wood Combustion; Slash Pine
95219	CNG Transit Bus Exhaust	P	CNG; Transit Bus Exhaust
95220	CNG Transit Bus Exhaust	P	CNG; Transit Bus Exhaust
95334	Diesel Exhaust - Heavy-heavy duty truck - 2011 model year	P	Diesel Exhaust; Heavy-heavy duty truck; 2011 model year; Ultra-low sulfur diesel
95429	Automated charbroiler - Hamburger	P	Automated charbroiler; Hamburger
95430	Underfired charbroiler - Hamburger	P	Underfired charbroiler; Hamburger
95431	Underfired charbroiler - Steak	P	Underfired charbroiler; Steak
95432	Underfired charbroiler - Chicken	P	Underfired charbroiler; Chicken
95433	Tire Dust	P	Tire Dust
95434	Tire Dust	P	Tire Dust
95435	Tire Dust	P	Tire Dust
95436	Tire Dust	P	Tire Dust
95437	Tire Dust	P	Tire Dust
95438	Tire Dust	P	Tire Dust
95439	Brake Wear	P	Brake Wear
95440	Brake Wear	P	Brake Wear
95441	Brake Wear	P	Brake Wear
95442	Brake Wear	P	Brake Wear
95443	Brake Wear	P	Brake Wear

Profile Number	Name	Profile Type	Keyword
95444	Brake Wear	P	Brake Wear
95445	Brake Wear	P	Brake Wear
95446	Brake Wear	P	Brake Wear
95447	Brake Wear	P	Brake Wear
95448	Brake Wear	P	Brake Wear
95449	Brake Wear	P	Brake Wear
95450	Brake Wear	P	Brake Wear
95451	Brake Wear	P	Brake Wear
95452	Brake Wear	P	Brake Wear
95453	Brake Wear	P	Brake Wear
95454	Brake Wear	P	Brake Wear
95455	Brake Wear	P	Brake Wear
95456	Brake Wear	P	Brake Wear
95457	Brake Wear	P	Brake Wear
95458	Brake Wear	P	Brake Wear
95459	Composite - Tire Dust	P	Composite; Tire Dust
95460	Composite - Tire Dust	P	Composite; Tire Dust
95461	Composite - Brake Wear	P	Composite; Brake Wear
95462	Composite - Brake Wear	P	Composite; Brake Wear

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APPENDIX B. Protocol for Expansion of SPECIATE Database

MEMORANDUM

Date: May 30, 2005

To: Lee Beck, U.S. Environmental Protection Agency, Office of Research and Development

From: Y. Hsu and S. Roe, E.H. Pechan & Associates, Inc.

Subject: Protocol for Expansion of the SPECIATE Database
EPA Contract No. 68-D-00-265, WA No. 4-46

This memorandum is intended to guide profile data collectors on how to collect and present source profile data to maximize their utility to SPECIATE users, to assist future SPECIATE managers in assessing whether the data should be incorporated, and to facilitate the process for preparing profiles in SPECIATE format.

Background

In order to ensure that future profile development meets the needs of the SPECIATE user community, the Workgroup has prepared several recommendations for speciation profile developers based on recent SPECIATE database updates and previous guidance from EPA (EPA, 2002) and other scientists (Watson and Chow, 2002). For this discussion, SPECIATE users are defined as individuals who: (1) conduct regional haze, $PM_{2.5}$, and ozone modeling; (2) prepare speciated emissions inventories; (3) use the Chemical Mass Balance or other receptor models; (4) and/or verify profiles derived from ambient monitoring measurements by multivariate receptor models such as UNMIX.

Speciation Data Collection

Profiles are defined as the weight percent of chemical species that make up a source-specific emission stream. Volatile organic compound (VOC) profiles should include the weight percent of each of the species present. When all organic gas species are present (e.g. methane, carbonyls, hydrocarbons), these profiles are referred to as total organic gas (TOG) profiles. At a minimum, these profiles should include the 56 Photochemical Assessment Monitoring Station (PAMS) species, as well as any other species that are available.

Particulate matter (PM) profiles should include the weight percent for each of the species present. Minimum data requirements are for the major elements reported by the IMPROVE and $PM_{2.5}$ Speciation Trends networks, water-soluble ions (sulfates and nitrates at a minimum, plus ammonium, potassium, sodium, chloride, fluoride, phosphate, calcium, and magnesium, if available), and carbon fractions [Total Carbon (TC), Organic Carbon (OC), and Elemental Carbon (EC)], preferably with other fractions that are defined by the method, such as the eight IMPROVE carbon fractions and carbonate carbon). Organic fractions, isotopic abundances, organic compounds, and single particle properties should be included, where they are reported and well-defined. Test results from dilution sampling trains are recommended for use in SPECIATE, since these results come closest to representing the composition of emissions in the ambient air.

Profile data must contain information on the chemical abundance of each species noted above. These data can be defined as the fraction of mass emissions of PM/VOC/TOG or the mass emission rate of each species (e.g. lb/ton, g/VMT, etc.). In addition to the estimate of central tendency for each species (e.g. mean, median), an estimate of the variability of each species should also be provided (e.g. standard deviation). Priority should be given to profiles that express the mean and standard deviation of individual test profiles for representative samples. If statistics other than the mean and standard deviation are provided, the method used to estimate central tendency and variability should be described.

Available information on the analytical uncertainty for individual test profiles should be identified and described separately. For example, if the analytical method for a certain species is known to have a precision of +/- 20%, then this information should be listed for each applicable species.

Documentation

The primary reference for the profile should be cited as the source of documentation, not secondary references that might have compiled profile data from one or more primary references. Secondary references should be cited only when original profiles have been modified (i.e. by aerosol aging, different sample compositing, different normalization methods, etc.). The notes column in the SPECIATE database should be used to store this information, as well as additional descriptive information on the profile, such as vehicle model year, engine size, vehicle identification number, and other descriptors that might be used to document a mobile source profile.

Profile developers must provide extensive documentation of their results. This should include documentation of the entire experimental program. Where appropriate, this should include fuel type, operating parameters, type of facility, location, and date of test. Non-detects or incomplete analyses should be documented so that the reader fully understands the analytical results.

Data Format

Profile developers should transmit data in a form that can be easily added to the SPECIATE database. The new SPECIATE 4.0 database is a Microsoft Access® relational database containing eight tables as described in Table C-1 of this appendix. The SPECIATE data structure is completely documented in the final report for SPECIATE 4.0. Information should be filled in as completely as possible, including references, test methods, analytical methods, Chemical Abstracts Service (CAS) numbers, data quality ratings, normalization basis, etc.

Data Normalization

Methods for profile normalization should be clearly documented, and the rationale for selecting the normalization basis should be stated. Normalization of organic gas data should be mass specific (i.e. mass species/mass TOG; emission rate species/emission rate TOG). Volume carbon basis is not recommended because it is objective (assumptions are needed regarding the composition of unresolved species). Whenever possible, the total gas chromatography (GC)-elutable organic gases normalization basis should be used and documented.

Normalization of PM data should be size-specific. Ideally, the profile will be normalized on total PM (with a specified upper size limit), PM_{10} and $PM_{2.5}$. However, normalization based on other size fractions can also be accommodated in SPECIATE. The normalized mass can be measured or be the weighted sum of major chemical components (sulfate, nitrate, ammonium, soil elements with assumed or measured oxides, organic carbon, elemental carbon, and sea salt). Profiles normalized on total gravimetric mass are preferred; however, if the sum of measured species basis is used, this should be noted and the reasoning for selecting this method stated.

Speciation Data Quality

Recommendations for or against inclusion of profiles in SPECIATE will be based on the perceived overall quality of the profiles. There are no simple criteria that can be set to scrutinize speciation data for inclusion in the SPECIATE 4.0 database. The supporting information housed within SPECIATE is therefore critically important. The SPECIATE 4.0 database provides structure sufficient to thoroughly document profiles and their underlying analysis, and should be completed as thoroughly as possible when preparing profiles for potential inclusion in the database.

Each profile has a quality rating that is assigned by the profile developer. The quality rating protocol is completely documented in the final report for SPECIATE 4.0. Speciation profiles developed from the following methods should be given a lower data quality rating:

1. Samples from combustion sources not collected by dilution sampling;
2. Low total speciated percentage (less than 80%);
3. PM profiles normalized by the "sum of species" mass, which assumes profiles of this type are fully speciated; and
4. Any noticeable outliers or other unreasonable test results (see examples provided below).

Additional profile quality considerations include:

- **Appropriate Method** – Reviewers experienced in analytical methods and application of speciation profiles will need to determine if characteristic compounds are present and properly measured. Sampling and analytical procedures need to be specific to the source and documented as thoroughly as possible. For example, the EPA Method TO-14 is not an appropriate method for dairy farm emission speciation. Since this method was developed to test industrial sources, fatty acids and other important organic species were not included in the target species list.

- **Measurement Precision** – Low precision is expected for certain species; the data quality ratings should reflect this issue. In cases where the sampling or analytical methods are found to be wholly inappropriate for a given species, these data should not be included in SPECIATE. For example, the wet chemistry using 2,4-Dinitrophenylhydrazine sampling procedure is not appropriate for acrolein measurement due to its poor recovery according to a study by California Air Resources Board (CARB) (Halm, 2003).

- **Overall Test Program Confidence** – Results obtained from the test program should be consistent with expectations for that source, and if not, the differences should be sufficiently accounted for. For example, in an U.S. Air Force sponsored study (AFIERA/RSEQ, 1998) measuring aircraft exhaust compositions, a brief discussion in the measurement section showed that the contractor measured essentially the same concentrations of target compounds in the background air as in the samples collected from aircraft exhaust. As a result, toxic species were reported at relatively low emission rates in this study. In cases where there are significant unexplainable results, the data should not be included in the SPECIATE database.

- **Source Category-specific Considerations** – For certain source categories such as the pulp and paper industry, oxygenated compounds contribute significantly to organic gas emissions. The generic total hydrocarbon (THC) method using flame ionization detectors (FID) calibrated with hydrocarbon standards (e.g. hexane) does not properly characterize the total TOG or VOC emissions. For processes whose emissions are dominated by methanol, this compound (and other oxygenated species) should be sampled and quantified separately using GC calibrated with a methanol standard (see Someshwar, 2003). Due to poor detector performance, the emission rates measured for THC were observed to be less than those measured specifically for methanol using an appropriate standard. Consequently, for this case, the THC is not suitable to serve as the normalization basis for this gas profile. The solution is to collect fully speciated data using appropriate methods and to consolidate all organic gases into a total organic gas profile for normalization.

References:

AFIERA/RSEQ, 1998. *Aircraft Engine and Auxiliary Power Unit Emissions Testing for the US Air Force*, Environmental Quality Management Inc, and Roy F. Weston Inc., December 1998.

EPA, 2002. *Draft Guidelines for the Development of Total Organic Compound and Particulate Matter Chemical Profiles*, developed by Emission Factors and Inventory Group, U.S. EPA, September 25, 2002.

Halm, 2003. Halm, C. of California Air Resources Board personal communication with Ying Hsu of E.H. Pechan & Associates, Inc., 2003.

Someshwar, 2003. Arun Someshwar, *Compilation of 'Air Toxic' and Total Hydrocarbon Emissions Data for Sources at Kraft, Sulfite and Non-Chemical Pulp Mills – an Update*, Technical Bulletin No. 858, National Council for Air and Stream Improvement, February, 2003.

Watson and Chow, 2002. Watson, J. and J. Chow, *Considerations in Identifying and Compiling PM and VOC Source Profiles for the SPECIATE Database*, Desert Research Institute, August, 2002.

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APPENDIX C. Speciation Profiles for Example Mixtures

Table C-1. SPECIATE Profile #3141 for Mineral Spirits

Chemical Name	Weight Percent	CAS
METHYLCYCLOHEXANE	9.80	108872
N-HEPTANE	5.10	142825
N-UNDECANE	4.47	1120214
N-DECANE	4.34	124185
TOLUENE	4.15	108883
N-OCTANE	3.86	111659
ACETONE	3.48	67641
CIS-1,3-DIMETHYLCYCLOHEXANE	2.46	638040
ETHYL ALCOHOL	2.37	64175
2-METHYLHEPTANE	2.18	592278
2,6-DIMETHYLNONANE	1.40	17302282
3-METHYLHEPTANE	1.38	589811
1,2,4-TRIMETHYLBENZENE {1,3,4-TRIMETHYLBENZENE}	1.38	95636
1,2,4-TRIMETHYLCYCLOPENTANE	1.33	99073
2-METHYLHEXANE	1.29	591764
TRANS,TRANS-1,2,4-TRIMETHYLCYCLOHEXANE	1.21	1678804
N-NONANE	1.17	111842
1,2-DIMETHYLCYCLOPENTANE	1.15	2452995
N-BUTYL ACETATE	1.14	123864
M-XYLENE	1.12	108383
ETHYL PROPYLCYCLOHEXANES	1.10	90090
ETHYLCYCLOHEXANE	1.01	1678917
4-METHYLNONANE	0.94	17301949
METHYL AMYL KETONE	0.86	110430
TRANS-1,4-DIMETHYLCYCLOHEXANE	0.85	2207047
TRANS-1,3-DIMETHYLCYCLOHEXANE	0.83	2207036
2-METHYLDECANE	0.83	6975980
METHYL PROPYLCYCLOHEXANES	0.82	26967646
2,6-DIMETHYLHEPTANE	0.76	1072055
3-METHYLDECANE	0.75	13151343
CIS-1,CIS-3,5-TRIMETHYLCYCLOHEXANE	0.69	1795273
1,2,3-TRIMETHYLCYCLOPENTANE	0.68	99074
TRANS,CIS-1,2,4-TRIMETHYLCYCLOHEXANE	0.67	99075
1,1,3-TRIMETHYLCYCLOPENTANE	0.66	4516692
1,1,3-TRIMETHYLCYCLOHEXANE	0.65	3073663
4-METHYLDECANE	0.64	2847725
1,2,3-TRIMETHYLBENZENE	0.63	526738
TRANS,TRANS-1,3,5-TRIMETHYLCYCLOHEXANE	0.63	99076
5-METHYLDECANE	0.63	13151354
4-METHYLHEPTANE	0.60	589537
BUTYLCYCLOHEXANE	0.58	1678939
N-DODECANE	0.57	112403

Table C-1 (continued)

Chemical Name	Weight Percent	CAS
2-METHYLNONANE	0.56	871830
ETHYLCYCLOPENTANE	0.56	1640897
TRANS-1,3-DIMETHYLCYCLOPENTANE	0.54	1759586
2,6-DIMETHYLOCTANE	0.54	2051301
5-METHYLINDAN	0.52	874351
1-METHYL-4N-PROPYLBENZENE	0.51	1074551
2,3-DIMETHYLOCTANE	0.49	7146603
BUTYL CELLOSOLVE {2-BUTOXYETHANOL} {EGBE}	0.48	111762
2,4-DIMETHYLHEXANE	0.45	589435
1-METHYL-4-ETHYLBENZENE	0.45	622968
4-METHYLOCTANE	0.45	2216344
2,5-DIMETHYLHEPTANE	0.44	2216300
3,7-DIMETHYLNONANE	0.44	17302328
CIS-1-ETHYL-3-METHYLCYCLOHEXANE	0.44	19489102
ETHYLBENZENE	0.43	100414
PROPYLCYCLOHEXANE	0.43	1678928
CIS-1,3-DIMETHYLCYCLOPENTANE	0.41	2532583
1-METHYLINDAN	0.41	767588
1-METHYL-3-ISOPROPYLBENZENE	0.41	535773
3-METHYLOCTANE	0.40	2216333
1,2,3-TRIMETHYLCYCLOHEXANE	0.40	1678973
OTHER C12	0.39	99035
METHYL ALCOHOL	0.37	67561
1-METHYL-2-ETHYLBENZENE	0.37	611143
2,5-DIMETHYLNONANE	0.37	17302271
P-XYLENE	0.35	106423
1-METHYL-3-ISOPROPYLCYCLOHEXANE	0.35	99040
1,2-DIMETHYL-4-ETHYLBENZENE	0.34	934805
3-METHYLNONANE	0.33	5911046
1-METHYL-3-ETHYLBENZENE	0.33	620144
O-XYLENE	0.32	95476
2,3-DIMETHYLHEXANE	0.32	584941
PENTYLCYCLOPENTANE	0.32	3741002
1-METHYL-2-ISOPROPYLCYCLOHEXANE	0.32	99041
3-ETHYLHEXANE	0.32	619998
2-METHYLOCTANE	0.31	3221612
OTHER C9	0.30	99032
ISOBUTYLCYCLOHEXANE	0.30	1678984
2-METHYLUNDECANE {ISODODECANE}	0.30	7045718
ISOPROPYLCYCLOHEXANE	0.29	696297
1,2,3,5-TETRAMETHYLBENZENE	0.29	527537
CIS,TRANS-1,2,4-TRIMETHYLCYCLOHEXANE	0.28	99079
1,3-DIMETHYL-2-ETHYLBENZENE	0.26	2870044
2,6-DIMETHYLDECANE	0.26	13150817
1,3-DIMETHYL-5-ETHYLBENZENE	0.26	934747
1,1-DIMETHYLCYCLOHEXANE	0.26	590669

Table C-1 (continued)

Chemical Name	Weight Percent	CAS
NAPHTHALENE	0.25	91203
ISOPROPYLBENZENE (CUMENE)	0.24	98828
DIETHYLCYCLOHEXANE	0.24	98062
2,4-DIMETHYLHEPTANE	0.23	2213232
TRANS-1-ETHYL-3-METHYLCYCLOHEXANE	0.23	99080
1,1,2-TRIMETHYLCYCLOPENTANE	0.22	4259001
1,2,4,5-TETRAMETHYLBENZENE	0.22	95932
1,4-DIMETHYL-2-ETHYLBENZENE	0.21	1758889
PENTYLCYCLOHEXANE	0.21	4292926
TRANS-1-ETHYL-4-METHYLCYCLOHEXANE	0.21	99082
INDAN	0.20	496117
3-ETHYL-2-METHYLHEPTANE	0.19	14676290
4,5-DIMETHYLOCTANE	0.19	15869962
1,1,3,4-TETRAMETHYLCYCLOHEXANE	0.18	99043
6-ETHYL-2-METHYLOCTANE	0.18	99044
3-PHENYLPENTANE	0.18	1196583
6-METHYLUNDECANE	0.18	99045
2,3-DIMETHYLPENTANE	0.17	565593
1-ETHYL-2-METHYLCYCLOPENTANE	0.17	99083
1-ETHYL-3-METHYLCYCLOPENTANE	0.17	99048
1,2-DIMETHYL-3-ETHYLCYCLOHEXANE	0.17	99046
CYCLOHEXANE	0.16	110827
3-ETHYLHEPTANE	0.16	15869804
4-ETHYLDECANE	0.16	99049
CIS-1,4-DIMETHYLCYCLOHEXANE	0.16	624293
OTHER C10	0.16	99033
3-METHYLHEXANE	0.15	589344
1-ETHYL-4-ISOPROPYLBENZENE	0.15	4218488
CIS-BICYCLO[4.3.0]NONANE	0.15	4551513
3,4-DIMETHYLHEXANE	0.15	583482
1,1,4-TRIMETHYLCYCLOHEXANE	0.15	7094271
1,3-DIMETHYL-4-ETHYLBENZENE	0.14	874419
OTHER C11	0.14	99034
3-ETHYL-3-METHYLOCTANE	0.14	99051
2-METHYLDECALIN	0.14	99050
3,6-DIMETHYLOCTANE	0.13	15869940
TRANS-1-ETHYL-2-METHYLCYCLOHEXANE	0.13	4923788
(2-METHYLBUTYL)CYCLOHEXANE	0.13	99052
1,2-DIETHYL-1-METHYLCYCLOHEXANE	0.13	99053
CIS,CIS-1,2,4-TRIMETHYLCYCLOHEXANE	0.13	99054
3-METHYLUNDECANE	0.13	1002433
1,3,5-TRIMETHYLBENZENE	0.12	108678
2,2,5-TRIMETHYLHEXANE	0.12	3522949
3,5-DIMETHYLOCTANE	0.12	15869939
4-METHYLUNDECANE	0.12	2980690
(1-METHYLPROPYL)BENZENE	0.11	135988

Table C-1 (continued)

Chemical Name	Weight Percent	CAS
5-METHYLUNDECANE	0.11	1632708
HEXYLCYCLOPENTANE	0.11	99057
5-ISOPROPYLNONANE	0.11	99056
2-ETHYL-1,3-DIMETHYLCYCLOHEXANE	0.11	99055
3,4-DIMETHYLOCTANE	0.11	15869928
3-ETHYLOCTANE	0.11	5881174
CIS-1,2-DIMETHYLCYCLOHEXANE	0.10	2207014
1,1-DIMETHYLCYCLOPENTANE	0.10	1638262
2,3,4-TRIMETHYLPENTANE	0.09	565753
2-METHYL-3-ETHYLPENTANE	0.09	609267
CIS,TRANS-1,2,3-TRIMETHYLCYCLOHEXANE	0.09	20348725
2,6-DIMETHYLUNDECANE	0.09	17301234
4-METHYLINDAN	0.09	824226
2,4-DIMETHYLPENTANE	0.08	108087
PROPYLCYCLOPENTANE	0.08	2040962
2,7-DIMETHYLOCTANE	0.08	1072168
1,1-DIMETHYL-2-PROPYLCYCLOHEXANE	0.08	99059
1-ETHYL-2,2,6-TRIMETHYLCYCLOHEXANE	0.08	99060
1,1-METHYLETHYLCYCLOPENTANE	0.07	16747505
1,1,2-TRIMETHYLCYCLOHEXANE	0.07	7094260
1-ETHYL-1,2-DIMETHYLCYCLOHEXANE	0.07	99061
TRANS-1,2-DIMETHYLCYCLOHEXANE	0.07	6876239
1,1,2,3-TETRAMETHYLCYCLOHEXANE	0.06	99062
3,3,5-TRIMETHYLHEPTANE	0.06	7154805
2,4-DIMETHYLNONANE	0.06	17302248
CIS-DECALIN	0.06	493016
1-ETHYL-2,4-DIMETHYLCYCLOHEXANE	0.06	99063
1-METHYL-4-ISOBUTYLBENZENE	0.06	99064
N-TRIDECANE	0.05	629505
3-ETHYLDECANE	0.05	17085960
CIS-1-ETHYL-2-METHYLCYCLOHEXANE	0.05	4923777
CIS-1-ETHYL-4-METHYLCYCLOHEXANE	0.05	3728561
CIS-BICYCLO[3.3.0]OCTANE	0.05	694724
4,5-DIMETHYLDECANE	0.05	99066
1,3-DIMETHYL-4-ISOPROPYLBENZENE	0.05	99065
1-METHYL-4-ISOPROPYLBENZENE	0.05	99876
N-PROPYLBENZENE	0.05	103651
2-METHYLNAPHTHALENE	0.04	91576
2,2,3,3-TETRAMETHYLPENTANE	0.04	7154792
CIS-1-ETHYL-2-METHYLCYCLOPENTANE	0.04	930892
OTHER C13	0.04	99037
2,5-DIMETHYLHEXANE	0.03	592132
1-METHYL-3-BUTYLBENZENE	0.03	99084
2,2-DIMETHYLHEPTANE	0.03	1071267
METHYL ISOBUTYL KETONE	0.03	108101
2,7-DIMETHYLDECANE	0.03	99067

Table C-1 (continued)

Chemical Name	Weight Percent	CAS
3,5-DIMETHYLNONANE	0.03	99068
2,3-DIMETHYLHEPTANE	0.03	3074713
OTHER C8	0.03	99031
N-BUTYL ALCOHOL	0.02	71363
3-ETHYL-4-METHYLHEPTANE	0.02	52896910
2,3,5-TRIMETHYLHEPTANE	0.02	20278857
1,1,3,5-TETRAMETHYLCYCLOHEXANE	0.02	4306654
HEXYLCYCLOHEXANE	0.02	4292755
TRANS-1-ETHYL-3-METHYLCYCLOPENTANE	0.02	99085
CIS-1-ETHYL-3-METHYLCYCLOPENTANE	0.02	99071
1,2,3-TRIMETHYL-4-ETHYLBENZENE	0.02	99070
OTHER C14	0.02	99038
STYRENE	0.02	100425
2,5-DIMETHYLOCTANE	0.02	15869893
METHYLCYCLOPENTANE	0.01	96377
2,4-DIMETHYLOCTANE	0.01	4032944
METHYL ETHYL KETONE (MEK) (2-BUTANONE)	0.01	78933
1-METHYL-4-ISOPROPYLCYCLOHEXANE	0.01	99821
METHYL PENTYLCYCLOHEXANE	0.01	99072

Table C-2. SPECIATE Profile #4439 for Xylene Mixtures

Chemical Name	Weight Percent	CAS
M-XYLENE	44.63	108383
O-XYLENE	19.82	95476
P-XYLENE	19.35	106423
ETHYL BENZENE	15.45	100414
TOLUENE	0.21	108883
1-ETHYL-3-METHYL BENZENE	0.15	620144
PROPYL BENZENE	0.15	98828
ISOPROPYL BENZENE	0.08	103651
1,2,4-TRIMETHYL BENZENE	0.06	95636
1-ETHYL-4-METHYL BENZENE	0.05	622968
1,3,5-TRIMETHYL BENZENE	0.03	108678
1-ETHYL-2-METHYL BENZENE	0.02	611143

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APPENDIX D. Semi-Volatile Organic Compound Partitioning Factors and Methodology Applied to Prepare Mobile Source Exhaust Profiles in the SPECIATE Database

MEMORANDUM

Date: September 3rd, 2007

To: Lee Beck, U.S. Environmental Protection Agency, Office of Research and Development

From: Ying Hsu, Ph.D. and Frank Divita Jr., Ph.D., E.H. Pechan & Associates, Inc.

Subject: Semi-volatile Organic Compound Partitioning Factors and Methodology Applied to Prepare Mobile Source Exhaust Profiles in the SPECIATE Database

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Introduction

This memorandum describes a method to allocate speciated semi-volatile organic compounds (SVOC) into estimates of particulate matter (PM) and organic gas phases. This procedure is required in order to convert SVOC emissions provided in speciation data into weight percent profiles.

Mobile source emission measurement studies frequently collect and analyze SVOC species in one sample. However, there is a need to separate their relative emissions because the current SPECIATE database defines speciation profiles as either PM or organic gas weight percent source profiles. The purpose of the memorandum is to propose a method to distribute measured SVOC species emission rates into PM and gas phases so that they can be normalized by particle and volatile organic compound* (VOC) emission rates and used in SPECIATE.

Methodology

To the best of Pechan's knowledge, after thorough literature review, there is only one motor vehicle study (Schauer et al., 1999) that comprehensively speciated diesel exhaust in PM and organic gas phases separately. Pechan proposes to apply the partitioning factors presented in the Schauer study to split SVOC species into PM and gas phases. For example, based on the Schauer's study (see Table 1), naphthalene (CAS # 91-20-3) is 100 percent gas phase under ambient condition, hexadecylcyclohexane (CAS # 6812-38-0) is entirely in the PM phase, and phenanthrene (CAS # 85-01-8) partitions 34 percent and 66 percent in PM and gas phase, respectively. For motor vehicle exhaust speciation data that measured SVOC that combined both PM and organic gas phases, Pechan will apply the partitioning factors in Table E-1 to allocate SVOC mass into in PM and gas phases.

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* The normalization basis can also be total organic gas (TOG) or non-methane organic gas (NMOG).

For example, when a study presents 0.67 mg/mile of naphthalene emission in both PM and gas phases, this emission rate is assumed to be entirely in gas phase and divided by organic gas mass emission rate and included in the associated organic gas profile. For phenanthrene, assuming the total emission rate is 0.0172 mg/mile, 34 percent of it (0.0059 mg/mile) is allocated in PM phase and 66 percent (or 0.0113 mg/mile) is in organic gas phase. These emission rates are then normalized by the associated PM and organic gas mass emissions, respectively.

Pechan understands partitioning factors are not universal and vary by sampling conditions (e.g., temperature, pressure). However, there are no better known protocols to allocate speciated SVOC emissions into PM and gas phases, once they are measured together. And, including SVOC species entirely in either PM phase or organic gas phase does not appropriately characterize motor vehicle emissions. For example, according to Schauer, et al. (1999), naphthalene is mostly in gas phase under ambient condition but it was estimated relative to PM emissions in an official mobile source emissions module. This is considered not appropriate since naphthalene is mostly in gas phase and not relevant to PM emissions.

Note: For integrity of this memorandum, excerpts from the Schauer, et al. (1999) study are briefly presented below. For complete details of this study, please consult the original reference below.

Excerpt from Mid-duty Diesel Exhaust Speciation Study by Schauer, et al. (1999)

Both gas- and particle-phase tailpipe emissions from medium duty diesel trucks were quantified using a two-stage dilution source sampling system. Tests were conducted in 1996 from in-use vehicle fleet in southern California and were fueled with commercially obtained California reformulated diesel fuel. The first vehicle tested was a 1995 model year Isuzu intercooled turbo diesel truck with a 3.8-L, four-cylinder engine. The second vehicle was a GMC Vandura 3500 full-sized commercial van with a 6.5-L, eight-cylinder diesel engine. The Isuzu truck and the GMC van had accumulated 39,993 miles and 30,560 miles of driving, respectively, prior to being tested.

Due to vehicle testing facility operating procedures, the diesel trucks could not be moved onto the dynamometer directly from cold storage. The truck had to be driven onto the dynamometer, which entailed first starting the engine, so the diesel trucks had to be tested with a hot-start Federal Test Procedure (FTP) cycle. Prior to the start of each source test, the truck tested was warmed on the dynamometer for approximately 10 minutes. The engine was then shut off, and the truck tailpipe was connected to the source sampler. The flows through the source samplers were established, and the truck was started and driven over the first two segments of the FTP dynamometer cycle.

The diesel trucks were driven through the hot-start FTP urban driving cycle on a transient chassis dynamometer. Emission rates of 52 gas-phase volatile hydrocarbons, 67 semivolatile and 28 particle-phase organic compounds, and 26 carbonyls were quantified along with fine particle mass and chemical composition. When all C1-C13 carbonyls were combined, they accounted for 60 percent of the gas phase organic compound mass emissions. Fine particulate matter emission rates and chemical composition were quantified simultaneously by two methods: a denuder/filter/PUF sampler and a traditional filter sampler. Both sampling techniques yielded the same elemental carbon emission rate of 56 mg/km driven, but the particulate organic carbon emission rate determined by the denuder-based sampling technique was found to be 35 percent lower than the organic carbon mass collected by the traditional filter-based sampling technique due to a positive vapor-phase sorption artifact that affected the traditional filter sampling technique. The distribution of organic compounds in the diesel fuel used in this study was compared to the distribution of these compounds in the vehicle exhaust. Significant enrichment in the ratio of unsubstituted polycyclic aromatic hydrocarbons (PAH) to their methyl- and dimethyl-substituted homologues was observed in the tailpipe emissions relative to the fuel. Isoprenoids and tricyclic terpanes were quantified in the semivolatile organics emitted from diesel vehicles. When used in conjunction with data on the hopanes, steranes, and elemental carbon emitted, the isoprenoids and the tricyclic terpanes may help trace the presence of diesel exhaust in atmospheric samples.

Reference

Schauer, et al., 1999: Schauer, J.J., M.J. Kleeman, G.R. Cass, and B.R.T. Simoneit, "Measurement of Emissions from Air Pollution Sources, 2. C1-C30 Organic Compounds from Medium Duty Diesel Trucks," Environmental Science and Technology, vol. 33, no. 10, pp. 1578-1587, 1999.

Table D-1. Average Emission Rates (µg/km) and Distribution of Organic Species in Medium Duty Diesel Truck Exhaust

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
1623	174.19	Octanedioic acid	505-48-6		138	0	1
936	188.22	Azelaic acid-TMS	123-99-9		176	0	1
1720	228.29	C1-MW 228 PAH			6.54	0	1
1620	270.45	Heptadecanoic acid	506-12-7		22.3	0	1
966	284.48	Stearic acid-TMS	57-11-4		362	0	1
959	298.50	Nonadecanoic acid-TMS	646-30-0		5.7	0	1
1730	308.59	Hexadecylcyclohexane	6812-38-0		12.9	0	1
1596	310.60	N-docosane	629-97-0		52.0	0	1
944	312.53	Eicosanoic acid-TMS	506-30-9		14.2	0	1
1731	322.62	Heptadecylcyclohexane	19781-73-8		16.7	0	1
1597	324.63	n-Tricosane	638-67-5		45.5	0	1
1732	336.64	octadecylcyclohexane	4445-06-1		11.5	0	1
1598	338.65	n-Tetracosane	646-31-1		40.7	0	1
1733	350.66	Nonadecylcyclohexane	22349-03-7		9.0	0	1
1599	352.68	n-Pentacosane	629-99-2		26.1	0	1
1600	366.71	N-hexacosane	630-01-3		34.9	0	1
1738	370.66	17 α(H)-22, 29, 30-trisnorhopane	53584-59-1		0.99	0	1
1846	370.66	18 α(H)-22, 29, 30- trisnorneohopane	55199-72-9		2.74	0	1
1736	372.68	20S-13β(H),17 α(H)-diacholestane	56975-84-9		1.37	0	1
1601	380.73	N-heptacosane	593-49-7		25.7	0	1
1602	394.76	n-octacosane	630-02-4		19.7	0	1
1725	398.72	17α(H), 21β(H),29-norhopane	53584-60-4		11.3	0	1
1603	408.79	n-Nonacosane	630-03-5		6.1	0	1
1726	412.74	17α(H), 21β(H)-hopane	13849-96-2		11.4	0	1
1744		20R&S-5 α(H), 14β(H), 17β(H)-ergostane			3.15	0	1
1745		20R&S-5 α(H), 14β(H), 17β(H)-sitostane			2.61	0	1

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
1743		20R-5α(H),14α(H),17α(H)-cholestane			1.19	0	1
1741		20R-5α(H),14β(H),17β(H)-cholestane			0.78	0	1
2336	228.29	Chrysene & Triphenylene	218-01-9; 217-59-4	3.35	15.6	0.177	0.823
1172	226.27	Benzo[ghi]fluoranthene	203-12-3	5.82	19.8	0.227	0.773
854	228.29	Benz(a)anthracene	56-55-3	2.98	7.76	0.277	0.723
1703	216.28	C1-MW 202 PAH		39.0	81.0	0.325	0.675
1173	228.29	Cyclopenta[cd]pyrene	27208-37-3	2.06	3.50	0.371	0.629
1702	202.25	Acephenanthrylene	201-06-9	12.0	16.2	0.426	0.574
1883	180.25	Methyl fluorene	26914-17-0	65.2	83.0	0.440	0.560
904	202.25	Pyrene	129-00-0	71.9	88.5	0.448	0.552
882	202.25	Fluoranthene	206-44-0	53.0	56.6	0.484	0.516
886	192.26	1-methylphenanthrene	832-69-9	17.0	17.8	0.489	0.511
1707	184.28	C4-naphthalenes		97.3	98.6	0.497	0.503
1701	220.31	C3-MW 178 PAH		97.4	97.5	0.500	0.500
1698	192.26	2-methylanthracene	613-12-7	10.4	10.4	0.500	0.500
1697	192.26	3-methylphenanthrene	832-71-3	30.3	29.4	0.508	0.492
1699	192.26	9-methylphenanthrene	883-20-5	22.9	22.0	0.510	0.490
852	178.23	Anthracene	120-12-7	12.5	10.9	0.534	0.466
889	192.26	2-methylphenanthrene	2531-84-2	42.0	35.6	0.541	0.459
1708	294.56	N-Pentadecylcyclohexane	6006-95-7	12.8	9.88	0.564	0.436
1595	296.57	N-heneicosane	629-94-7	65.8	40.5	0.619	0.381
1706	170.25	C3-naphthalenes		240	130	0.649	0.351
902	178.23	Phenanthrene	85-01-8	93.1	47.0	0.665	0.335
1042	282.55	Eicosane	112-95-8	206	95.7	0.683	0.317
1845	332.61	8β,13α-dimethyl-14β- [3'-methylbutyl]-podocarpane		13.8	4.50	0.754	0.246
1700	206.28	C2-MW 178 PAH		196	57.2	0.774	0.226
881	180.20	9-fluorenone	486-25-9	34.6	9.84	0.779	0.221
883	166.22	Fluorene	86-73-7	34.6	9.5	0.785	0.215

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
1718	266.51	tridecylcyclohexane	6006-33-3	16.5	4.34	0.792	0.208
1843	280.53	Tetradecylcyclohexane	1795-18-2	15.9	3.96	0.801	0.199
1709	137.19	8β,13α-dimethyl-14β-n-butylpodocarpane		44.0	10.6	0.806	0.194
873	168.19	Dibenzofuran	132-64-9	28.7	6.0	0.827	0.173
1729	136.15	Methylbenzoic acid	12167-74-7	772	26.7	0.967	0.033
1045	226.44	Hexadecane	544-76-3	711	8.62	0.988	0.012
1043	240.47	Heptadecane	629-78-7	614	5.92	0.990	0.010
1690	212.41	2,6,10-Trimethyldodecane (farnesane)	3891-98-3	434	4.1	0.991	0.009
1047	268.52	Nonadecane	629-92-5	411	3.82	0.991	0.009
1693	226.44	Norpristane	3892-00-0	566	4.9	0.991	0.009
1049	212.41	Pentadecane	629-62-9	398	2.12	0.995	0.005
1602	394.76	n-octacosane	630-02-4	601	2.84	0.995	0.005
1692	226.44	2,6,10-trimethyltridecane	3891-99-4	367	1.2	0.997	0.003
282	26.04	Acetylene	74-86-2	4600		1	0
452	28.05	Ethylene	74-85-1	8560		1	0
465	30.03	Formaldehyde	50-00-0	22300		1	0
678	42.08	Propylene	115-07-1	780		1	0
279	44.05	Acetaldehyde	75-07-0	41800		1	0
46	54.09	1,3-butadiene	106-99-0	310		1	0
283	56.06	Acrolein (2-propenal)	107-02-8	3400		1	0
367	56.11	Cis-2-butene	590-18-1	260		1	0
497	56.11	Isobutylene	115-11-7	1140		1	0
737	56.11	Trans-2-butene	624-64-6	520		1	0
839	58.04	Glyoxal	107-22-2	2100		1	0
673	58.08	Propionaldehyde	123-38-6	14000		1	0
592	58.12	N-butane	106-97-8	3830		1	0
391	68.12	Cyclopentene	142-29-0	210		1	0
382	70.09	Crotonaldehyde	4170-30-3	13400		1	0
188	70.09	2-methyl-2-propenal	78-85-3	4000		1	0
181	70.13	2-methyl-1-butene	563-46-2	260		1	0
230	70.13	3-methyl-1-butene	563-45-1	160		1	0
390	70.13	Cyclopentane	287-92-3	410		1	0

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
742	70.13	Trans-2-pentene	646-04-8	50		1	0
1464	72.06	Methylglyoxal	78-98-8	1700		1	0
313	72.11	Butyraldehyde (butanal)	123-72-8	1300		1	0
536	72.11	Methyl ethyl ketone (2-butanone)	78-93-3	7500		1	0
508	72.15	Isopentane	78-78-4	2740		1	0
605	72.15	N-pentane	109-66-0	1860		1	0
302	78.11	Benzene	71-43-2	2740		1	0
187	84.16	2-methyl-2-pentene	625-27-4	210		1	0
369	84.16	Cis-2-hexene	7688-21-3	100		1	0
385	84.16	Cyclohexane	110-82-7	210		1	0
551	84.16	Methylcyclopentane	96-37-7	620		1	0
740	84.16	Trans-2-hexene	4050-45-7	160		1	0
1463	86.09	Biacetyl	431-03-8	900		1	0
122	86.18	2,2-dimethylbutane	75-83-2	310		1	0
136	86.18	2,3-dimethylbutane	79-29-8	570		1	0
199	86.18	2-methylpentane	107-83-5	930		1	0
248	86.18	3-methylpentane	96-14-0	670		1	0
717	92.14	Toluene	108-88-3	3980		1	0
550	98.19	Methylcyclohexane	108-87-2	520		1	0
840	100.16	Hexaldehyde	66-25-1	2200		1	0
140	100.20	2,3-dimethylpentane	565-59-3	720		1	0
152	100.20	2,4-dimethylpentane	108-08-7	410		1	0
194	100.20	2-methylhexane	591-76-4	570		1	0
245	100.20	3-methylhexane	589-34-4	310		1	0
600	100.20	N-heptane	142-82-5	470		1	0
301	106.12	Benzaldehyde	100-52-7	3800		1	0

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
449	106.17	Ethylbenzene	100-41-4	470		1	0
522	106.17	M-xylene & p-xylene	108-38-3; 106-42-3	2330		1	0
620	106.17	O-xylene	95-47-6	830		1	0
1018	114.19	Heptanal	111-71-7	3200		1	0
118	114.23	2,2,4-trimethylpentane	540-84-1	1240		1	0
130	114.23	2,3,4-trimethylpentane	565-75-3	310		1	0
138	114.23	2,3-dimethylhexane	584-94-1	160		1	0
149	114.23	2,4-dimethylhexane	589-43-5	50		1	0
156	114.23	2,5-dimethylhexane	592-13-2	50		1	0
193	114.23	2-methylheptane	592-27-8	100		1	0
226	114.23	3-ethylhexane	619-99-8	210		1	0
604	114.23	N-octane	111-65-9	260		1	0
1013	118.13	2,3-benzofuran	271-89-6	53.2		1	0
976	120.15	Acetophenone	98-86-2	5100		1	0
30	120.19	1,2,4-trimethylbenzene (1,3,4-trimethylbenzene)	95-63-6	880		1	0
44	120.19	1,3,5-trimethylbenzene	108-67-8	260		1	0
89	120.19	1-Methyl-3-ethylbenzene	620-14-4	210		1	0
608	120.19	N-propylbenzene	103-65-1	100		1	0
94	120.19	1-Methyl-4-ethylbenzene	622-96-8	520		1	0
937	122.12	Benzoic acid-TMS	65-85-0	1260		1	0
611	128.17	Naphthalene	91-20-3	617		1	0
1065	128.21	Octanal	124-13-0	3100		1	0
603	128.26	N-nonane	111-84-2	160		1	0
1713	132.16	1-Indanone	83-33-0	69.5		1	0
1712	134.18	2,5-Dimethylbenzaldehyde	5779-94-2	4100		1	0
105	142.20	1-Methylnaphthalene	90-12-0	378		1	0
196	142.20	2-methylnaphthalene	91-57-6	611		1	0
1057	142.24	Nonanal	124-19-6	4400		1	0

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
1617	144.21	Octanoic acid	124-07-2	125		1	0
847	152.19	Acenaphthylene	208-96-8	70.1		1	0
846	154.21	Acenaphthene	83-32-9	19.3		1	0
657	154.29	Pentylcyclohexane	4292-92-6	83.9		1	0
1801	156.22	C2-Naphthalenes		542		1	0
997	156.27	Decanal	112-31-2	2800		1	0
1618	158.24	Nonanoic acid	112-05-0	240		1	0
480	168.32	Hexylcyclohexane	4292-75-5	14.9		1	0
1658	170.29	Undecanal	112-44-7	2600		1	0
599	170.33	N-dodecane	112-40-3	503		1	0
941	172.26	Decanoic acid-TMS	334-48-5	72.9		1	0
1840	182.35	Heptylcyclohexane	5617-41-4	20.0		1	0
1714	184.26	Dibenzothiophene	132-65-0	1.98		1	0
1659	184.32	Dodecanal	112-54-9	1200		1	0
609	184.36	N-tridecane	629-50-5	477		1	0
1619	186.29	Undecanoic acid	112-37-8	206		1	0
909	196.20	Xanthone	90-47-1	12.4		1	0
1841	196.37	Octylcyclohexane	1795-15-9	26.2		1	0
1660	198.34	Tridecanal	10486-19-8	2000		1	0
1051	198.39	Tetradecane	629-59-4	629		1	0
1691	198.39	Norfarnesane	6864-53-5	360		1	0
954	200.32	Lauric acid-TMS, or dodecanoic acid	143-07-7	58.5		1	0
1694	210.40	N-Nonylcyclohexane	2883-02-5	24.7		1	0
970	214.34	Tridecanoic acid-TMS	638-53-9	13.1		1	0
1695	224.43	Decylcyclohexane,	1795-16-0	38.2		1	0
958	228.37	Myristic acid-TMS, or n-Tetradecanoic Acid	544-63-8	5.3		1	0
1716	238.45	Undecylcyclohexane	54105-66-7	23.9		1	0
1717	252.48	Dodecylcyclohexane	1795-17-1	16.8		1	0
1704	268.53	Pristane	1921-70-6	443		1	0

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
1705	282.55	Phytane	638-36-8	439		1	0
2337	332.50	2,2'-Dithiobisbenzothiazole	120-78-5	251		1	0