Final Report

SPECIATE Version 5.0
Database Development Documentation

June 2019

EPA Contract No. EP-BPA-17H-0012
EPA/600/R-19/098

Submitted to:
Dr. Marc Menetrez (E343-02)
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

Submitted by:
Abt Associates Inc.
Drs. Ying Hsu, Frank Divita, and Jonathan Dorn
6130 Executive Boulevard
Rockville, MD 20852-4907

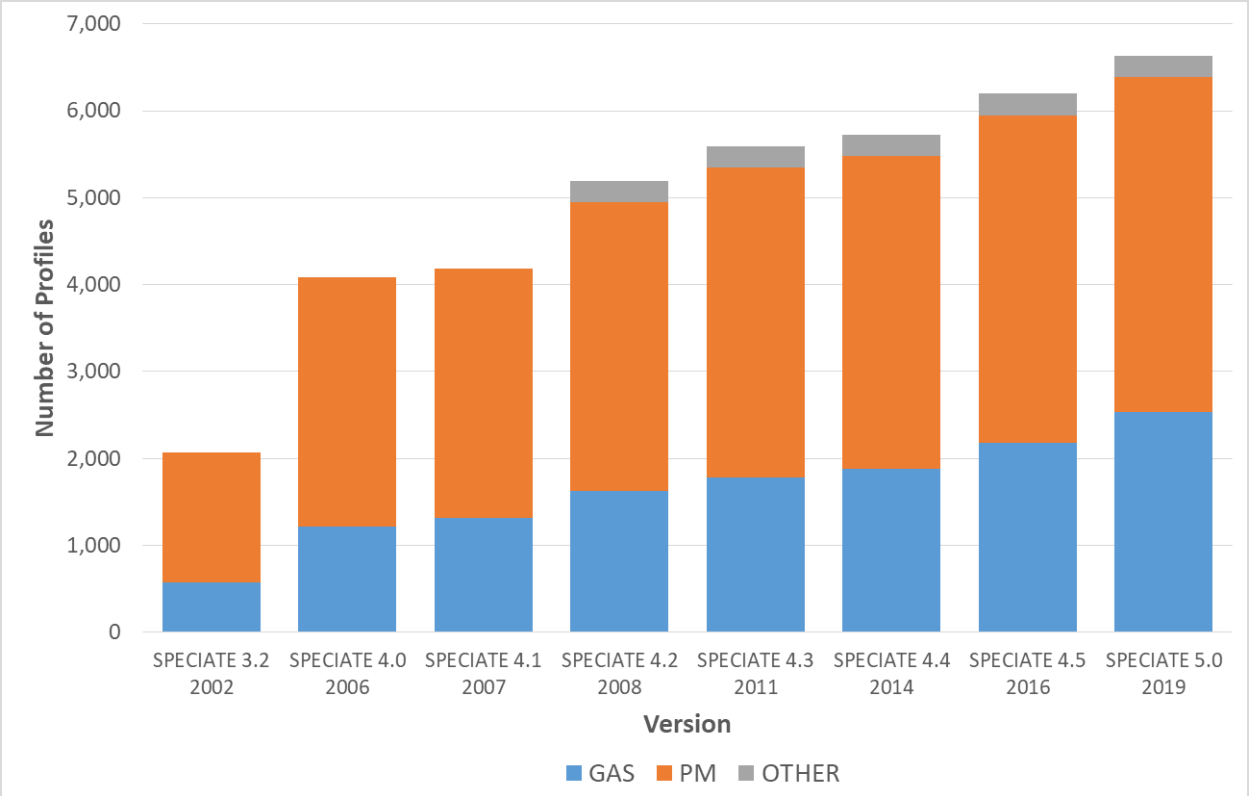
Executive Summary

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of speciation profiles of air pollution sources that provide the species makeup or composition of organic gas, particulate matter (PM) and other pollutants emitted from these 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) developing black carbon assessments and particulate carbonaceous inventories; (3) estimating air toxic pollutant emissions from PM and organic gas primary emissions; (4) providing input to chemical mass balance (CMB) receptor models; and, (5) verifying profiles derived from ambient measurements by multivariate receptor models (e.g., factor analysis and positive matrix factorization).

EPA routinely uses SPECIATE data for development of air quality modeling platforms and for the National Emissions Inventory (NEI). For the NEI, SPECIATE data are used to estimate black carbon (elemental carbon) emissions and other species of PM and to estimate hazardous air pollutants (HAPs) for some source categories.

SPECIATE 3.2, released in 2002, was the first electronic version, a Microsoft Access® database. Periodically, EPA releases an updated version of SPECIATE that adds data to previous versions of the Microsoft Access® database. EPA also provides the data in a browser tool to allow users to browse and download profile information without the need to use Microsoft Access®. EPA is now releasing SPECIATE 5.0.

The figure below shows the number of profiles added to the various releases of SPECIATE.



The development and update of SPECIATE is accomplished by a multi-office EPA Speciate Workgroup (SWG) comprised of staff from the Office of Research and Development (ORD) and Office of Air and Radiation (OAR) from the following laboratories and offices:

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

SWG members select the data, quality assure the data and profiles, and coordinate on improvements to the database structure and metadata fields. As newer SPECIATE versions are developed, improvements are made to the process as well as the data.

Processes that have been improved in SPECIATE include the method by which the SWG evaluates profiles for inclusion, a systematic approach to identify profile needs, updates to reference information, and improved documentation.

EPA generated SPECIATE 5.0 by appending 370 organic gas profiles and 86 PM profiles to the SPECIATE 4.5 database. In total, the SPECIATE 5.0 database includes 6,654 profiles. The organic gas profiles added span a large number of different sources including oil and gas, biomass burning, mobile sources and consumer products. The PM profiles include various combustion sources and dust. Some of the sources complemented sources already in SPECIATE, other sources such as speciation from oil and gas ponds, and sugar cane burning were new to SPECIATE. EPA added model-ready versions of existing SPECIATE PM profiles to support aerosol modules currently available and being developed.

EPA made structural improvements to the SPECIATE 5.0 database to consolidate common fields and tables. EPA expanded the metadata fields to include additional information on profile quality and to collect data that would support the volatility basis set approach for air quality models. Additional species properties such as vapor pressure which facilitates gas/particle partitioning were added.

The SPECIATE BROWSER has been improved in capability, accessibility, and usability. Users can search for profiles by any of the fields associated with a profile or the species contained in the profile.

Adding profiles to SPECIATE requires many layers of review including processes to prioritize and evaluate the data. For SPECIATE 5.0 an additional quality assessment scoring system (resulting in a quality score or QSCORE) was developed to evaluate profiles using criteria that cuts across many aspects of profile development and potential use such as measurement techniques, completeness and source category needs.

Through the development of SPECIATE 5.0, ideas for continued future improvements and directions have been discussed by the SWG. These are included in Chapter VI of this document.

In summary, the maintenance of SPECIATE requires continuous assessment. EPA SWG members have established a process to identify and prioritize need, find sound research sources which address that need, critically review those sources, and finally add that data to SPECIATE. This rigorous attention to maintaining quality and relevance has established SPECIATE as a uniquely positioned source of information for air quality analysts, modelers, researchers, specialists, as well as interested public officials and individuals.

This report first discusses the uses and structure of the SPECIATE 5.0 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. Chapter VI provides future directions and is followed by references and appendices.

Acknowledgments

SPECIATE 5.0 is made possible by the following organizations that fund and/or provide employee resources:

- 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 (SWG) and those individuals that provided data for the SPECIATE 5.0 database. The primary contact for the project is Dr. Marc Menetrez, the EPA Task Order Contract Officer Representative (TOCOR) for this project; the Alternate TOCOR is Dr. Madeleine Strum. The SWG is coordinated by Dr. Menetrez and staffed by air quality professionals from the EPA's Office of Research and Development (ORD) and the Office of Air and Radiation (OAR). As of May 2019, the committee members include:

SPECIATE WORKGROUP MEMBERSHIP, May 2019			
NAME	EPA OFFICE	EPA DIVISION	EXPERTISE/SPECIALIZATION
Souad Benromdhane	OAR/OAQPS	HEID	Health Benefits of Air Quality Management
Casey Bray	OAR/OAQPS	SPPD	Emission Source Speciation
Justine Geidosch	OAR/OTAQ	ASD	Mobile Source Emissions
Ingrid George	ORD/NRMRL	AEMD	Emission Source Testing and Black Carbon
Michael Hays	ORD/NRMRL	AEMD	Emission Source Testing
Brooke Hemming	ORD/NCEA	NCEA-RTP	Climate Change and Black Carbon
Amara Holder	ORD/NRMRL	AEMD	Emission Source Testing and Black Carbon
Marc Menetrez	ORD/NRMRL	AEMD	Emission Source Speciation
Ben Murphy	ORD/NERL	CED	Secondary Organic Aerosol Modeling
Libby Nessley	ORD/NRMRL	AEMD	QA Manager
George Pouliot	ORD/NERL	CED	Emissions Modeling (Inventories and Platforms)
Havala Pye	ORD/NERL	CED	Secondary Organic Aerosol Modeling
Momei Qin	ORD/NERL	CED	Secondary Organic Aerosol Modeling
Venkatesh Rao	OAR/OAQPS	AQAD	Biomass Burning, Black Carbon Inventory and Agricultural sources
Heather Simon	OAR/OAQPS	AQAD	Air Quality Modeling
Madeleine Strum	OAR/OAQPS	AQAD	National Emissions Inventory and Emissions Modeling
Tiffany Yelverton	ORD/NRMRL	AEMD	Air Pollution Control, Combustion, and Black Carbon

CONTENTS

LIST OF TABLES

LIST OF FIGURES

Acronyms and Abbreviations

AAAR	American Association for Aerosol Research
ACS	American Chemical Society
AEMD	Air and Energy Management 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	Community Multi-scale Air Quality Modeling System
CMB	chemical mass balance
CRC	Coordinating Research Council
CTM	chemical transport model
DOE	Department of Energy
DRI	Desert Research Institute
EC	elemental carbon
EF	emission factor
ERMD	Emissions Research and Measurement Division (Environment Canada)
EPA	Environmental Protection Agency
ES&T	Environmental Science and Technology
FID	flame ionization detector
GC	gas chromatography
GHG	greenhouse gas
HAPs	hazardous air pollutants
HDDV	heavy-duty diesel vehicle
HEID	Health and Environmental Impacts Division, EPA
ID	identification
IO	immediate office
ITN	internal tracking number
IVOC	intermediate volatile organic compounds
kg	kilogram
km	kilometer
LDDV	light-duty diesel vehicle
LVOC	low volatility organic compound
LVP	low vapor pressure
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
NMHC	non-methane hydrocarbons
NMOG	non-methane organic gas
NPRI	National Pollutant Release Inventory (Environment Canada)
NREL	National Renewable Energy Laboratory
NRMRL	National Risk Management Research Laboratory, EPA
OAQPS	Office of Air Quality Planning and Standards, EPA
OAR	Office of Air and Radiation, EPA

OC	organic carbon
OM	organic matter
ORD	Office of Research and Development, EPA
OTAQ	Office of Transportation and Air Quality, EPA
QSCORE	profile quality score
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
POC	primary organic compounds
POA	primary organic aerosols
RFG	reformulated gasoline
RTP	Research Triangle Park
SAROAD	Storage and Retrieval of Aerometric Data
SIC	Standard Industrial Classification
SMOKE	Sparse Matrix Operator Kernel Emissions (EPA emissions modeling tool)
SOA	secondary organic aerosol
SRS	Substance Registry System
SVOC	semi-volatile organic compounds
SWG	SPECIATE work group
TAME	t-amylmethyl ether
TAP	toxic air pollutant
TC	total carbon
TCEQ	Texas Commission on Environmental Quality
THC	total hydrocarbon
TOCOR	Task Order Contract Officer Representative
TOG	total organic gases
TOR	thermal optical reflectance
TOT	thermal optical transmission
UV	ultraviolet-visible
VBS	volatility basis set
VOC	volatile organic compounds

CHAPTER I. Introduction

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of organic gas and particulate matter (PM) speciation profiles of air pollution sources (Simon et al., 2010, Simon et al., 2018). A speciation profile provides the chemical composition of an emission source in weight percent of PM or organic gas. Organic gas profiles may represent total organic gases (TOG), volatile organic compounds (VOC) or a variation as described further in Chapter 2, Section C. PM speciation profiles include data for PM of various size classes, such as $PM_{2.5}$, which represents the mass of particles less than or equal to 2.5 microns in diameter. In addition to PM and organic gas profiles, SPECIATE contains other profiles such as for nitrogen oxides, mercury and semi-volatile organic compounds (SVOC).

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 by metadata to document the source of data. There are instances where multiple profiles are available for the same source type. In these cases, the SWG develops composite profiles to better represent the emission source compositions (see Chapter IV, Section M for a description of composite profiles).

Speciation profiles are used by EPA, other governmental and non-governmental agencies including international agencies, the regulated community, and academia for a number of purposes such as: (1) creating speciated emissions inventories for regional haze, PM, greenhouse gas (GHG), and photochemical air quality modeling; (2) developing black carbon assessments and particulate carbonaceous inventories; (3) estimating air toxic pollutant emissions from PM and organic gas primary emissions; (4) providing input to chemical mass balance (CMB) receptor models; and, (5) verifying profiles derived from ambient measurements by multivariate receptor models (e.g., factor analysis and positive matrix factorization).

EPA routinely uses SPECIATE data for development of air quality modeling platforms and for the National Emissions Inventory (NEI). For the NEI, SPECIATE data are used to estimate black carbon (elemental carbon) emissions and other species of PM and to estimate hazardous air pollutants (HAPs) for some source categories.

Periodic updates are made to 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, 4.5, and 5.0) allow for storage of important information underlying each profile (metadata such as sampling and analysis methods, normalization procedures, profile quality ratings, etc.). SPECIATE profiles are never removed from the database, and often multiple profiles exist for a source type representing different levels of control, operating conditions, locations, etc.

The SWG consists of EPA staff who meet regularly to contribute and/or gather data and provide recommendations as to which specific speciation profiles should be added to the database. They also evaluate the profiles to be added and provide quality assurance (QA) for the database and documentation prior to the release of the data.

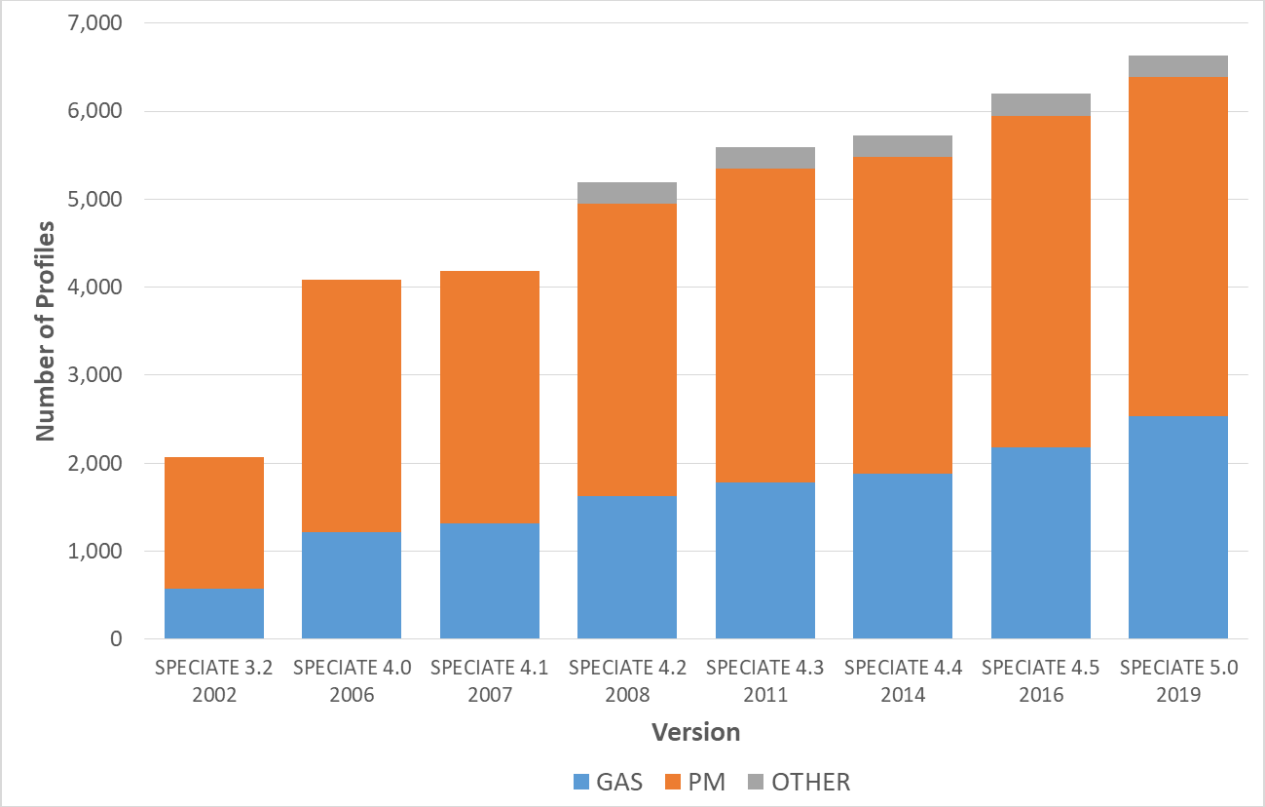
The SPECIATE 3.2 database, which was released in 2002 was the first electronic version, a Microsoft Access® database, and contained profiles that are the result of testing and/or studies conducted in the 1980s, and in some cases, the 1970s. EPA released an updated SPECIATE database version 4.0 in November 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, 4.5 and 5.0. The purpose of this report is to document the updates that EPA applied to SPECIATE 4.5 to generate the SPECIATE 5.0 database.

The SPECIATE 5.0 database can be downloaded from the EPA website:

https://www.epa.gov/air-emissions-modeling/speciate *(last accessed April 2019)*

Figure 1 shows how the database has increased in profiles throughout the versions since the first electronic version, SPECIATE 3.2

Figure 1. Profiles Added to the Various Releases of SPECIATE



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 for modeling 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 gas profiles (now referred to as "OTHER"). This category contains speciated mercury, nitrogen oxides, and SVOC which do not fall into VOC or PM profile categories. There are 237 OTHER 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 AE6 aerosol module in the Community Multi-scale Air Quality (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 data can be used to support other mechanisms in additional air quality models.

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.

SPECIATE 4.5 (2016) 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. This database also includes "model-ready"[1] PM profiles following the method described in Reff et al. (2009).

SPECIATE 5.0 (2019) adds 370 gas profiles and 86 PM profiles which include 13 profiles to support the volatility basis set (VBS) approach in air quality modeling. In addition, 212 species (that were contained in the consumer products profiles added to SPECIATE 5.0) are added. The database updates include major structural changes by merging common tables (PM, Gas, OTHER profiles) into one PROFILES table. Similarly, the PM_SPECIES, GAS_SPECIES, and OTHER_SPECIES tables are combined into the SPECIES table, and KEYWORD and REFERENCE tables into the KEYWORD_REFERENCE table. Additional information of the SPECIATE 5.0 data tables can be found in Figure 3 and Table 1. As part of the structural changes, the SWG also added multiple new metadata fields, e.g., categorization fields, to assist users searching for profiles, master pollutant emission rate, an additional profile quality score (QSCORE), species emission rate for all profile types, organic matter to organic carbon ratio, and mass overage (associated with reconstructed PM mass). For each chemical specie, vapor pressures and carbon to oxygen ratios were added. Corrections were made to the NonVOCTOG data field to properly characterize those species (such as siloxanes) that are exempt per the regulatory definition of VOC but were incorrectly characterized as VOC in previous versions of the database. In addition, SPECIATE 5.0 provides the workbooks used to translate the data from the original source into the SPECIATE profile format for uploading into the database. Workbooks can be downloaded from EPA's SPECIATE page https://www.epa.gov/air-emissions-modeling/speciate *(last accessed April 2019).*

Figure 2 depicts 'The Flow Chart for Evaluating the Addition of Speciation Profiles to the SPECIATE Database.' It lists a step-by-step pathway of responsibilities for identifying and evaluating source emissions study findings for inclusion into SPECIATE. Figure 2 illustrates the many layers of review and process facilitation that documents the evaluated quality of prioritized profiles going into SPECIATE. The process starts when a library search is conducted by library staff under the direction of the EPA SWG members. Keywords and cursory quality directives are used to isolate relevant literature. Literature is then

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

screened by SWG members and feedback is often requested and received from the SWG and EPA at large. Publications are sought which describe and document research studies of organic gas and respirable PM speciation profiles of air pollution sources which meet the highest standards of quality assessment, completeness, reproducibility, represent well planned and conducted efforts, and address areas of research designated as important to SPECIATE. Unusable publications are discarded at this point as well as after additional reviews are conducted (Bray et al. 2017 and Simon et al. 2018).

An initial review is conducted by EPA and Abt and usable publications are passed along for further evaluation; unusable publications are discarded. Potentially usable publications or other data sources are entered in a "Master Evaluation" spreadsheet for further prioritization. Figure 2 also depicts those functions that are currently shared between the EPA SWG group and the contractor (yellow highlight). Those potentially usable publications will undergo the generation of a workbook, once selected by the SWG. The workbook is an accompanying compendium of data from each profile, organized and made available for later review and data use efforts. If the publication covers multiple experiments or sources, the workbook may include multiple profiles. It may also include a composite across different experiments or sources that average the data across individual experiments or sources.

The initiative to update SPECIATE to Version 5.0 produced the following total number of profiles and unique species:

- 6,654 PM, GAS, and OTHER profiles;
- 2,814 unique species; and
- 198 PM-AE6 profiles.

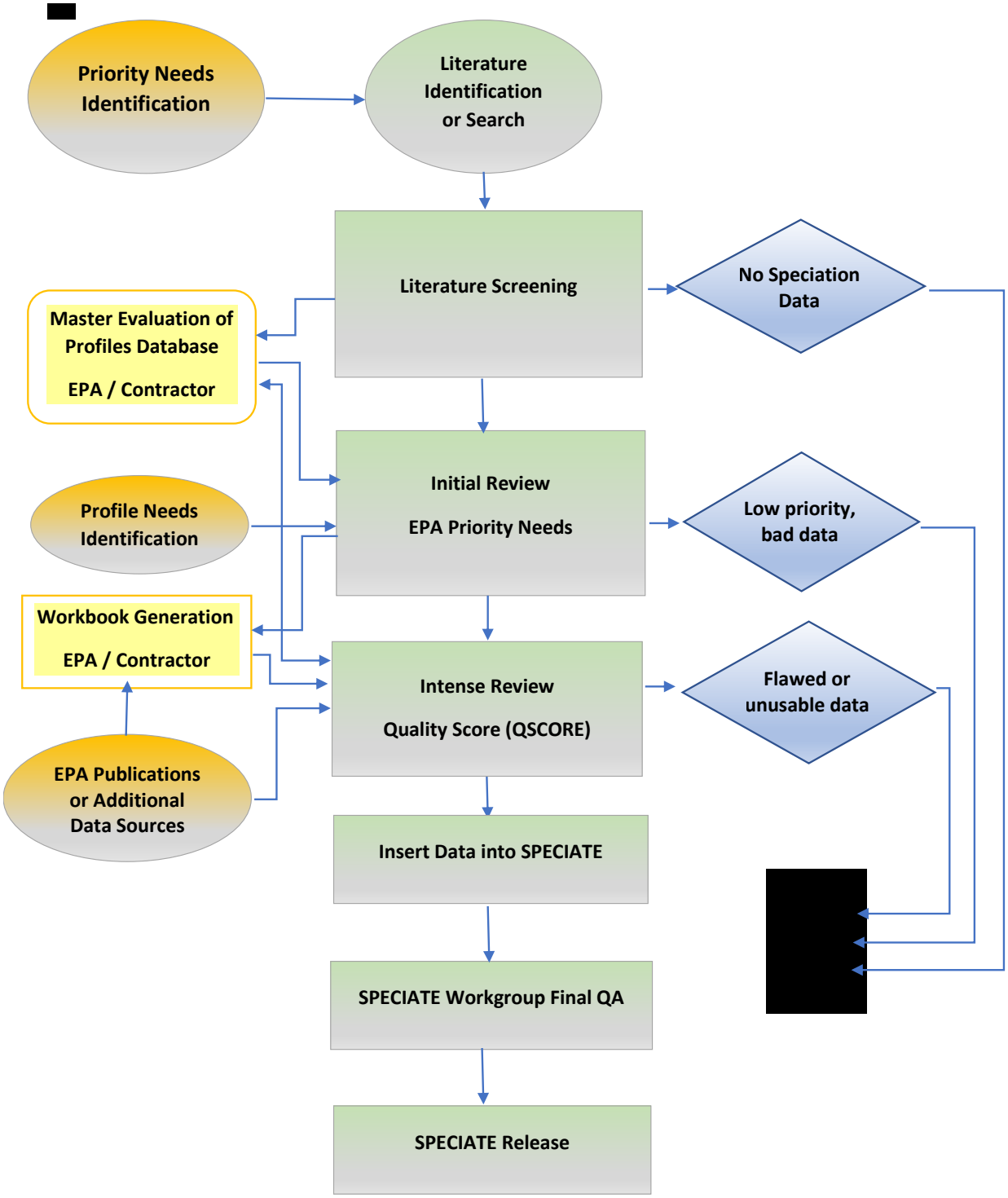
  Note: PM-AE6 profiles are used as inputs to the aerosol module of the CMAQ photochemical model (see Appendix G for details).

In addition to the Microsoft Access® SPECIATE database, EPA provides the workbooks and additional documentation (in cases where a published reference or internet-accessible report is not available) on the SPECIATE page of the air emissions modeling platform website, https://www.epa.gov/air-emissions-modeling (*last accessed April 2019)*.

SPECIATE is an ongoing project that supports EPA research, scientific assessments, regulation development and enforcement. The SWG 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 https://www.epa.gov/air-emissions-modeling/forms/contact-us-about-air-emissions-modeling *(last accessed April 2019)*.

The remainder of this report discusses the new structure and use of the SPECIATE 5.0 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 added to the SPECIATE 5.0 database, respectively. Appendix B provides the original protocol for preparing profiles for the future versions of the SPECIATE database that was used to support earlier versions. 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. Appendix E outlines the QSCORE evaluation framework which is meant to guide the reviewer to assign quality value points to the areas of the study deemed most important for use in SPECIATE. Appendix F summarizes three profile categorization fields. Appendix G describes the protocol for developing AE6-ready $PM_{2.5}$ speciation profiles for inclusion in SPECIATE.

Figure 2. Flow Chart for Evaluating the Addition of Speciation Profiles to the SPECIATE Database



CHAPTER II. SPECIATE Database

This chapter describes the organization of the SPECIATE 5.0 database. This includes subsections on the use of the database, the data dictionary, profile quality rating criteria, and profile categorization.

A. Use of the Database

The SPECIATE 5.0 database is a data repository housed in a Microsoft Access® database file that contains the new profiles from the current SPECIATE 5.0 process and all previous versions. In order to use the SPECIATE 5.0 database, Microsoft Access 2002® or a newer version must be installed. The current SPECIATE database and other relevant documentation can be downloaded from EPA's Air Emissions Modeling website. https://www.epa.gov/air-emissions-modeling (*last accessed April 2019*). The direct link to the SPECIATE page is: https://www.epa.gov/air-emissions-modeling/speciate *(last accessed April 2019).* To facilitate inspection of the data by persons without detailed database manipulation skills, queries are available that link the key PROFILES, SPECIES, SPECIES_PROPERTIES, and KEYWORD_REFERENCE tables together to allow the user to view the fields in these tables when the queries are run. The View_GAS_Profiles query has a filter to display the organic gas profiles [TOG, reactive organic gas (ROG), VOC, non-methane organic gas (NMOG), and non-methane hydrocarbons (NMHC)]. The View_PM_Profiles query allows the user to view all PM profiles.

The data may also be obtained through the SPECIATE 5.0 data browser on EPA's SPECIATE webpage, where all fields in the SPECIATE database are provided. This new web-based data browser, designed using the Qlik® platform (https://www.qlik.com/us), allows users to view and filter profile data, including the weight percents of species, from any metadata field and export selected records into Microsoft Excel®. In addition, users of the browser can create custom tables that provide only the fields of interest and can view profile weight percents for individual profiles in a stacked bar chart format for visualization and comparisons across profiles.

B. Database Design

The SPECIATE 5.0 database design appears in Figure 3. 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.

The PROFILE_TYPE field distinguishes between different types of profiles. Previous versions of SPECIATE had "GAS" profiles "PM" profiles and "OTHER GAS" (mercury, NOx, SVOC). Additional types were added in SPECIATE 5.0 to delineate those that are associated with specific air quality modeling aerosol parameterizations, and "OTHER GAS" was changed to "OTHER." The SPECIATE 5.0 database has PROFILE_TYPE values of: GAS, PM, OTHER, PM-SIMPLIFIED, PM-AE6, PM-VBS and GAS-VBS. These are described in the data dictionary (Subsection C).

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 PROFILES 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 5.0 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.

The use of PROFILE_CODE as the primary key for the profiles table 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 PROFILES 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 a GAS profile have been developed from the same study, the SIBLING field is used to identify the associated profiles.

The fields UNCERTAINTY_PERCENT, UNCERTAINTY_METHOD, and ANALYTICAL_METHOD (see Table 1 and subsection C below) in the SPECIES table store species-specific uncertainty values, uncertainty methods, and analytical methods, respectively.

Figure 3. SPECIATE 5.0 Data Diagram

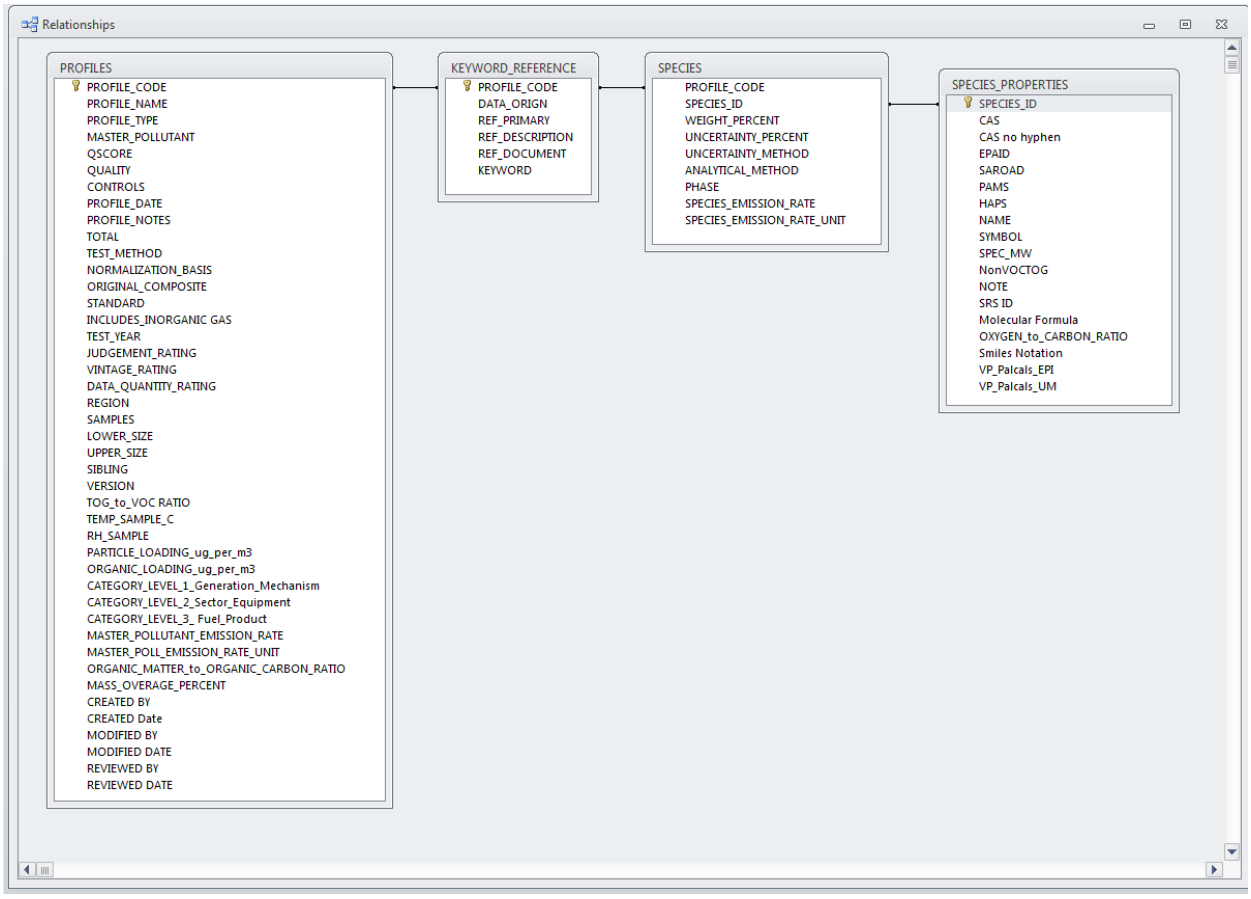


Table 1. Descriptive Data Dictionary

Field Name	Data Type	Length[1]	Description
PROFILES Table			
PROFILE_CODE	Text	10	Profile Code - alphanumeric. Ideally less than 7 characters for mobile profiles and less than 10 characters for others due to emissions model (e.g., SMOKE) field length limitations
PROFILE_NAME	Text	255	Profile Name
PROFILE_TYPE	Text	20	Indicates type of profile: PM-AE6, PM-VBS, PM-Simplified, PM, GAS, GAS-VBS and OTHER
MASTER_POLLUTANT	Text	25	Indicates the pollutant to be used in calculation.
QSCORE	Number	2	Profile quality score out of 30 points total. 20-30 = excellent. 12-19 = good. 5-11 = fair. Less than 5 = poor.
QUALITY	Text	3	Overall Quality Rating (A-E) based on Vintage Rating and Data Quantity Rating, see Chapter II.D for an explanation
CONTROLS	Text	150	Emission Controls Description
PROFILE_DATE	Date/Time	10	Date profile added (MM/DD/YYYY)
PROFILE_NOTES	Memo		Notes about the source and how data were put together. Examples include method for compositing, descriptions about the overall procedures and/or study purpose
TOTAL	Number	6	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).
TEST_METHOD	Memo		Description of sampling/test method for overall profile
NORMALIZATION_BASIS	Text	100	Description of how profile was normalized (see Chapter IV.F for details)
ORIGINAL_COMPOSITE	Text	2	Specifies whether the profile is original, composite of SPECIATE profiles or study composite. Allowed values: 'C','O','SC'. The option for study composite, SC, added in SPECIATE5.0, means composite was developed in the study.
STANDARD	Yes/No	1	Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
INCLUDE_INORGANIC GAS	Yes/No	1	Indicates the presence or absence of inorganic gas species in this profile (e.g., sulfur dioxide, hydrogen sulfide, oxides of nitrogen, etc.)
TEST_YEAR	Text	50	Indicates year testing was completed
JUDGEMENT_RATING	Number	4	Subjective expert judgement rating based on general merit (see Chapter II.D for an explanation)
VINTAGE_RATING	Number	4	Vintage based on TEST_YEAR field (see Chapter II.D for an explanation)

Field Name	Data Type	Length[1]	Description
DATA_QUANTITY_RATING	Number	4	Data sample size rating based on number of observations, robustness (see Chapter II.D for an explanation)
REGION	Text	50	Geographic region of relevance
SAMPLES	Text	255	Number of samples (separate experiments or measurements) used to make the profile.
LOWER_SIZE	Number	5	Identifies lower end of aerodynamic diameter particle size, micrometers
UPPER_SIZE	Number	5	Identifies upper end of aerodynamic diameter particle size, micrometers
SIBLING	Text	25	GAS or PM Profile number taken from the same study, if exists
VERSION	Text	5	SPECIATE database version that a profile was added to
TOG_to_VOC RATIO	Number	6	Ratio of TOG mass to VOC mass, computed as: 100%/(100%-sum(nonVOC)%)
TEMP_SAMPLE_C	Number	6	Temperature while samples were taken, in degrees Celsius
RH_SAMPLE	Number	6	Relative humidity while samples were taken.
PARTICLE_LOADING_ug_per_m3	Number	6	PM loading during sampling in units of micrograms/m^3
ORGANIC_LOADING_ug_per_m3	Number	6	Organic loading during sampling in units of micrograms/m^3
CATEGORY_LEVEL_1_Generation_Mechanism	Text	255	The mechanism by which emissions are generated by the emissions source. (See Appendix F for details)
CATEGORY_LEVEL_2_Sector_Equipment	Text	255	This category provides more detail on the emissions generation category by including the sector and/or equipment or process used to generate the emissions. (See Appendix F for details)
CATEGORY_LEVEL_3_ Fuel_Product	Text	255	This category provides the highest level of detail for the profile categorization. (See Appendix F for details)
MASTER_POLLUTANT_EMISSION_RATE	Number	6	PM or GAS emission rate, if available
MASTER_POLLUTANT_EMISSION_RATE_UNIT	Text	50	PM or GAS emission rate units, if available
ORGANIC_MATTER_to_ORGANIC_CARBON_RATIO	Number	4	OM/OC ratio to calculate OM emissions. OM/OC ratio of 1.25 for motor vehicle exhaust, 1.4 for coal combustion, 1.7 for biomass combustion (other than wood fired boilers), 1.4 for wood fired boilers and all others, with some exceptions.
MASS_OVERAGE_PERCENT	Number	6	Sum of species percentages that is over 100% calculated only for PM_AE6 profiles for which the mass of the measured OC and computed PNCOM was reduced so that the AE6 profile would not exceed 100%
CREATED BY	Text	50	Person who added this profile
CREATED DATE	Date/Time		Date the profile was added
MODIFIED BY	Text	50	Person who modified this profile
MODIFIED DATE	Date/Time		Date the profile was added

Field Name	Data Type	Length[1]	Description
REVIEWED BY	Text	50	Person who reviewed this profile
REVIEWED DATE	Date/Time		Date the profile was reviewed
SPECIES Table			
PROFILE_CODE	Text	10	Unique Identifier links to PROFILES table.
SPECIES_ID	Number	5	Species Identifier (Same as in SPECIES_PROPERTIES table)
WEIGHT_PERCENT	Number	6	Weight percent of pollutant (%)
UNCERTAINTY_PERCENT	Number	6	Uncertainty percent of pollutant (%)
UNCERTAINTY_METHOD	Memo	64	Description of method used to calculate uncertainty
ANALYTICAL_METHOD	Text	100	Description of analytical method (e.g., X-ray fluorescence spectroscopy, ion chromatography)
PHASE	Text	50	Indicate whether emissions were measured for PM, gaseous, or both phases.
SPECIES_EMISSION_RATE	Number	6	Species emission rate
SPECIES_EMISSION_RATE_UNIT	Text	50	Species emission rate units (e.g., mg/mile)
KEYWORD_REFERENCE Table			
PROFILE_CODE	Text	10	Unique Identifier links to PROFILES table.
DATA_ORIGN	Text	50	Source of data (e.g., EPA Air Pollution Prevention and Control Division (APPCD), Schauer, CARB, DRI, NPRI, Literature)
REF_PRIMARY	Yes/No		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.
REF_DESCRIPTION	Memo		Stores the descriptive information about the profile.
REF_DOCUMENTS	Memo		Complete reference citation. Some profiles have multiple citations such as reports and journal articles.
KEYWORD	Text		Keywords describing a profile.
SPECIES_PROPERTIES Table			
SPECIES_ID	Number	9	Unique Identifier (Link to SPECIES table)
CAS	Text	50	Chemical Abstracts Service (CAS) number assigned to pollutant (with hyphens) (blank if no CAS)
EPA_ID	Text	50	EPA Chemical Identifier; provided by EPA Substance Registry System (SRS) for species without CAS numbers
SAROAD	Text	5	Storage and Retrieval of Aerometric Data (SAROAD) code
PAMS	Yes/No	1	Is PAMS pollutant? (Yes or No)

Field Name	Data Type	Length[1]	Description
HAPS	Yes/No	1	Is Hazardous Air Pollutant (HAP)? (Yes or No) HAPs are defined in in the Clean Air Act, Section 112(b), changes to that list are in the Code of Federal Regulations (CFR), Title 40, Part 63, see https://www.epa.gov/haps/what-are-hazardous-air-pollutants for current list.
NAME	Text	255	Species Name
SYMBOL	Text	9	Standard chemical abbreviation
SPEC_MW	Number	6	Species molecular weight
NonVOCTOG	Yes/No	1	Is this species regarded as a volatile organic compound (VOC)? The VOC definition is from 40 CFR. §51.100
NOTE	Memo	250	Note (notes) about the SPECIES_ID or its properties
SRS ID	Text	50	EPA SRS Chemical Identifier
Molecular Formula	Text	50	Molecular formula
OXYGEN_to_CARBON_RATIO	Number		Ratio of oxygen atoms to carbon atoms
Smiles Notation	Text	10	Smiles notation
VP_Pascal_EPI	Number		Vapor Pressure in units of Pascals from the EPISUITE model (recommended by SWG member Ben Murphy, EPA/ORD/NERL)
VP_Pascal_UM	Number		Vapor Pressure in units of Pascals from UManSysProp tool (uses the EVAPORATION algorithm, slightly updated) http://umansysprop.seaes.manchester.ac.uk/tool/vapour_pressure

1 Length – maximum number of characters allowed.

C. Data Dictionary

The SPECIATE 5.0 database is a Microsoft Access® relational database containing four tables as described in Table 1 and Figure 3.

- The PROFILES table includes, but is not limited to, profile code, name, notes on the profile, and descriptive information about the profile.
- The PROFILES table has a distinct set of profile types (see Table 2) (fieldname is PROFILE_TYPE). A profile would be in only one of these categories: GAS, PM, OTHER, PM-SIMPLIFIED, PM-AE6, PM-VBS and GAS-VBS. Profiles with type equal to "PM-SIMPLIFIED" are $PM_{2.5}$ profiles that support the AE5 Aerosol Module in CMAQ; PM-AE6 profiles are $PM_{2.5}$ profiles that support the AE6 aerosol module in CMAQ. PM-AE6 profiles include additional species that are not typically measured such as PNCOM and particulate water. A protocol to create a PM-AE6 profile is provided in Appendix G. Two new profile types, GAS-VBS and PM-VBS were added to SPECIATE 5.0, though there are very few actual profiles of these types. These few VBS profiles are introduced in SPECIATE5.0 at the same time the CMAQ VBS aerosol mechanism is being developed by EPA/ORD researchers. This has helped to identify database needs to support additional metadata and to set the stage for producing additional VBS-profiles in future SPECIATE versions. PM profiles (without the dash) are any PM profile that is not one of the other categories and was the original type of all PM profiles prior to creating PM profiles that are "model ready" in SPECIATE. The profile types are defined below.

Table 2. Description of PROFILE types

Profile Type	Definition
GAS	Organic gas profiles. They can be TOG, NMOG, THC, VOC, and NMHC profiles, depending on the available species and analytical methods.
GAS-VBS	Organic gas profiles to support the volatility basis set (VBS) approach in air quality modeling such as CMAQ. These are typically profiles for which the raw measurement data are aggregated and/or non-measured species are derived from the measured species.
PM	Particulate matter (PM) profiles include data for PM of various size classes, such as $PM_{2.5}$, which represents the mass of particles from 0 to 2.5 microns in diameter.
PM-SIMPLIFIED	$PM_{2.5}$ profiles that support the AE5 Aerosol Module in CMAQ.
PM-AE6	$PM_{2.5}$ profiles that support the AE6 aerosol module in CMAQ. PM-AE6 profiles include additional species that are not typically measured such as PNCOM and particulate water.
PM-VBS	PM profiles to support the VBS approach in air quality modeling.
OTHER	OTHER profiles are those that do not fit in the organic gas or PM categories. Examples of the OTHER profiles are nitrogen oxides (nitric oxide (NO), nitrogen dioxide (NO_2), nitrous acid (HONO)) and speciated mercury (elemental and oxidized mercury).

- Gas profiles can be TOG, NMOG, THC, VOC, and NMHC profiles, depending on the available species and analytical methods. Information on whether the profile is for TOG, NMOG, VOC, NMHC is provided in the MASTER_POLLUTANT field. TOGs are compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate. VOC contain similar compounds as TOGs, except VOC 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 *(last accessed April 2019).*

  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, and other compounds listed in the regulatory definition of VOC provided below).

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 compounds of carbon that participate in atmospheric photochemical reactions, excluding methane, ethane, acetone, carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate. VOC, additionally, exclude numerous exempt compounds that can be found in the Electronic Code of Federal Regulations under Title 40, Chapter I, Subchapter C, Part 51, Subpart F,§51.100. A direct link is here: http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8.

The list of exempt compounds is updated when new compounds are added through rulemaking.

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 gas chromatography-flame ionization detector (GC-FID). Notably, an FID measures carbon and hydrogen.

NMOG = NMHC + oxygenated compounds

- The PROFILES table also contains OTHER profiles. OTHER profiles are those that do not fit in the organic gas or PM categories. Examples of the OTHER profiles are nitrogen oxides (nitric oxide (NO), nitrogen dioxide (NO_2), nitrous acid (HONO)) and speciated mercury (elemental and oxidized mercury).
- The SPECIES table includes the species identification number, the profile code 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 KEYWORD_REFERENCE table includes keywords and 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). This table includes descriptive keywords of profiles. This information can be used in keyword-based searches for profiles.
- The SPECIES_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 Quality 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 SWG 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 SWG 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 Judgement Rating (expert judgement) 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:

- *VINTAGE 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 2006-Present, score = 5. The data are housed in the VINTAGE RATING field in the PROFILES table.
- *DATA QUANTITY 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. The data are housed in the DATA QUANTITY RATING field in the PROFILES tables.
- QUALITY (*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 "VINTAGE RATING" x "DATA QUANTITY RATING." Table 3 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 3. 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 N 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 VINTAGE RATING or DATA QUANTITY RATING (or JUDGEMENT 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.

JUDGEMENT RATING (expert judgement) – 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 the sum of species may have only targeted specific compounds and may therefore not be complete.);
- Supporting documentation;
- Source of data (e.g. highly-regarded 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 JUDGEMENT RATING. These inherently qualitative values are assigned by the principal investigator for profiles obtained from the DRI, by Abt Associates technical staff, or per the guidance of the SWG. EPA SWG 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, JUDGEMENT 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 judgement 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.

For the new profiles added to the SPECIATE 5.0 database, the SWG has developed a new quality rating field called QSCORE (Quality SCORE) in the PROFILES table. The QSCORE provides an evaluation framework to easily recognize and assign value points to indicators of a strong, well planned and executed study, which is presented in a complete and logical manner. A point to each question adds-up to an evaluation score. An ideal score would have a total of 30 (Data from Measurements) or 29 (Data from other Methods) points. Each point or points is additive, influencing, but not necessarily distinguishing the study. The publication or report should be ranked as high as possible for inclusion into the SPECIATE database. The QSCORE total points are valued as follows:

20-30 = excellent
12-19 = good
5-11 = fair
<4 = poor

Each QSCORE is added to the PROFILES table in the SPECIATE Database. See Appendix E. Profile Quality Criteria Evaluation.

E. Profile Categorization

The SWG added three profile categorization fields to the PROFILES table to provide readily searchable metadata about the emission source covered by the profile. The fields describe the emission source in terms of emission generation mechanism (level 1), sector and/or equipment (level 2) and fuel and/or product (level 3). These categorization fields are added to help users to identify and group profiles from similar sources and search for profiles. The categorization has been developed for use in the downstream processing of PM speciation profiles for air quality modeling. Currently, profiles for the AE6 mechanism

for CMAQ must be created manually and then put into SPECIATE. Efforts have begun to enhance the Speciation Tool, a software program which creates model-ready profiles for input into emissions modeling software, to create AE6 mechanism profiles. This tool will use the profile category fields to assign the appropriate organic matter to organic carbon ratio (OM-to-OC ratio) which is necessary for computing the species needed for AE6 PM profiles. This ratio is dependent on the type of source and could be assigned using the three categorization fields (See Appendix F. Description of Three Profile Categorization Fields).

CHAPTER III. Profiles Included in SPECIATE

Speciation data and profiles obtained from EPA, California Air Resources Board (CARB), DRI, Texas Commission on Environmental Quality (TCEQ), Environment Canada, Coordinating Research Council (CRC), National Renewable Energy Laboratory (NREL), and numerous peer-reviewed journal articles were considered for inclusion in the SPECIATE 4.0 through 5.0 databases.

A list of new speciation profiles added to the SPECIATE 5.0 database, as of May 2019, 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 SWG obtained profiles. Subsection A contains new speciation profiles included in the SPECIATE 5.0 database. All other subsections in this chapter identify the profiles carried forward from the SPECIATE 4.0 through 4.5 databases.

During the development of the SPECIATE database, the SWG identified hundreds of peer-reviewed journal articles and technical reports to evaluate for use in developing profiles for SPECIATE. The SWG prioritized the datasets, with the highest priority given to EPA data as well as the data selected for SPECIATE 5.0 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, the SWG continues to prepare 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. An initial protocol for expansion of the database was originally developed to support an earlier version of SPECIATE and is presented in Appendix B. A separate document "SPECIATE: Guidelines for Data Developers" was developed using Appendix B as a starting point and is available on the SPECIATE webpage. These guidelines help engage and inform the research community about the content and quality consideration of data so that the EPA can consider these data for inclusion into SPECIATE.

A. New Profiles Included in SPECIATE 5.0

SPECIATE 5.0 includes new profiles from EPA, CARB, Wyoming Department of Environmental Quality, DRI, and the scientific literature. Some of these are discussed here.

The EPA SWG developed multiple TOG profiles with gap filled methane and ethane for poultry production, beef cattle and swine farm emissions. EPA prepared AE6 versions of profiles in previous versions of SPECIATE such as for a ship auxiliary engine burning marine gas oil and a profile for forest fires. EPA added a corrected version of a heavy-duty diesel exhaust profile (EPA does not remove SPECIATE profiles from previous versions, so the original profile remains with metadata changes). Roy et al investigated the relationship between ambient temperature and the compositions of gasoline vehicular exhaust emissions (Roy et al. 2016) and profiles were added based on this work. CARB has a speciation database that contains profiles they developed based on surveyed wide categories of consumer products and architectural coatings in California. These profiles were adapted for SPECIATE 5.0 by further speciating the mixtures. These product-type-specific profiles along with more general composites were added. DRI conducted the "Lake Tahoe Source Characterization Study" and developed a suite of road dust and residential wood combustion profiles using multiple woods as fuel for fireplaces and woodstoves; these were added to SPECIATE. They also collaborated with other researchers to publish PM profiles burning corn stalk, rice, and wheat straw in China which were added. The PM profiles developed by University of Wisconsin at Madison who studied soils and road dust in in the Midwestern U.S. were added. Coal combustion PM profiles using different coals and published data in the literature

were added. Utah State University investigated composition and fluxes of organic gas from oil and gas production wastewater ponds and generated numerous TOG profiles which were added. Wyoming Department of Environmental Quality shared their oil and gas test data and assisted EPA in using them to construct county-specific profiles for SPECIATE 5.0. Other profiles added to the database are small off-road engine exhaust tested on leaf blowers, trimmers, soil tillers, and lawnmowers. Work was also done by incorporating and combining the measurements of two sugar cane burning studies to construct sugar cane burning profiles for TOG; these data were also used to create HAP emission estimates for the NEI. A complete set of SPECIATE 5.0 profiles can be obtained from the database by filtering the VERSION field to 5.0.

B. Additional EPA Speciation Data

In addition to the above profiles added to the SPECIATE 5.0 database, other 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), gap-filled TOG profiles based on the Hays SPECIATE4.0 VOC profiles added to SPECIATE5.0;
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); a composite of these added to SPECIATE 5.0;
21. The effects of operating conditions on semi-volatile organic compounds emitted from light-duty, gasoline-powered motor vehicles (Herrington et al., 2012; PM profiles, added to SPECIATE 4.4).
22. Speciation Profiles and Toxic Emission Factors for Nonroad Engines (EPA-420-R-14-028; TOG profiles, added to SPECIATE 4.5);
23. 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, added to SPECIATE 4.5);
24. Tribal Minor Source Registration Data, Region 8 - Uintah & Ouray Indian Reservation (EPA Region 8; TOG profiles, EPA 2015a, added to SPECIATE 4.5);
25. WRAP Phase III oil and gas speciation profiles (WRAP Phase III Support Data; TOG profiles, added to SPECIATE 4.5);
26. Oil and Natural Gas Flare profiles (Shah, et. al; TOG profiles added to SPECIATE4.5)
27. CNG Transit Bus Exhaust (EPA-420-R-15-022, EPA, 2015b; PM profiles, added to SPECIATE 4.5);
28. Carbonaceous Aerosols Emitted from Light-Duty Vehicles Operating on Gasoline and Ethanol Fuel Blends (Hays et al., 2013; PM profiles);
29. Three model year 2011 heavy-duty on-highway diesel engines were characterized for regulated and unregulated emissions using the FTP and the 16-Hour. A composite profile was added to SPECIATE 4.5 and correction to remove alcohols added to SPECIATE5.0 (Imad et al. 2011);
30. Spark-Ignition Exhaust Emissions from 2-stroke off-road engines - Non-oxygenated gasoline added to SPECIATE 4.5 (Reichle et. al, 2015);
31. Diesel Exhaust Emissions from Tier 2 Off-road Engines was added to SPECIATE 4.5 (Cook et al, 2015).

C. University Research Group Speciation Data

Researchers associated with 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 SWG. 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.

Researchers, Schauer et al. and Rogge et al., conduct studies that are extremely detailed in that they speciated hundreds of organic compounds in PM, in addition to ions, metals, elemental carbon (EC) and 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, 2018). These profiles are used by CARB during the development of state implementation plans, TAP emission inventories, photochemical modeling, receptor modeling, and other air quality projects.

In previous versions of SPECIATE (prior to SPECIATE 5.0), 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.

In SPECIATE 5.0, 107 CARB profiles were added to update the consumer products and architectural coatings profiles added in previous versions. The consumer products profiles are from the 2010 update, and the architectural coatings are from the 2005 survey. All of these use a profile code that begins with "CARB" and follows with the profile identifier used by CARB in their speciation profile database. In addition, several composite profiles were developed using weighting factors from CARB emissions inventories.

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 (DOE) funded Gasoline-Diesel PM Split Study (DOE, 2005) were included in the SPECIATE 4.2 database. An additional set of fireplace wood burning and road dust profiles for the California Lake Tahoe Source Characterization Study (Kuhns, et al., 2004) were added to the SPECIATE 5.0 database.

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

As recommended by the SWG, 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, and 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).

In May 2009, the TCEQ contracted with The University of Texas at Austin to conduct the Comprehensive Flare Study project (TCEQ, 2011). The purpose of this project was to conduct field tests to measure flare emissions and collect process and operational data in a semi-controlled environment to determine the relationship between flare design, operation, vent gas lower heating value and flow rate, destruction and removal efficiency, and combustion efficiency. These data were utilized by Shah, et. al to develop flare profiles for SPECIATE 4.5.

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

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 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 a Microsoft 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°C and 20°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 CO, NO_x, THC, NMHC, 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 (CRC) 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 onroad 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 SWG raised issues and questions regarding the SPECIATE database. This chapter describes results and recent decisions made by the SWG.

A. SPECIATE Database Needs Assessment

SPECIATE 5.0 contains speciation profiles for most emission sources. However, the SWG continuously strives to search for speciation data that are more specific for source types, processes, and different regions. A needs analysis was performed on the most prominent emission source profiles applied in EPA's 2014 version 7.0 air emissions modeling platform which used version 1 of the 2014 National Emissions Inventory (US EPA, 2018a; US EPA, 2016). To identify and prioritize profiles most in need of updating the authors developed a ranking system based on six major criteria (Bray et al., 2019): (1) representativeness of current technology (i.e. does the tested emission source still represent the current technology?), (2) the level of documentation (e.g. peer reviewed, report, etc.), (3) the appropriateness of the source category codes to which profiles are applied, (4) prevalence in the EPA modeling platform,(5) any additional known problems with the profile or the data provided in the original reference or in the SPECIATE database, and (6) applicability of study region. Higher scoring profiles are those with higher priority need for improvements (Bray et al., 2019). The results of this work found that the most common concern for profiles in need of updates is their appropriateness for the sources to which they are applied. Many of these mapping mismatches are due to lack of emissions testing for appropriate source categories. The needs assessment ranking system identified $PM_{2.5}$ profiles for wildfires, agricultural burning, heavy-duty diesel vehicle exhaust (which is being applied to nonroad diesel equipment), sub-bituminous coal combustion and nonroad gasoline exhaust as the highest priority $PM_{2.5}$ profiles in need of new data. For VOC, it was found that a wide range of VOC emissions are assigned to the overall average, as specific profiles do not exist. Examples of source sectors where speciation data profiles are needed include oil and gas industry (extraction wells, dehydration sumps, processing plants, storage tanks, distribution and transmission leaks), household and yard waste burning, pulp and paper industry boiler combustion, consumer products, architectural and industrial maintenance coating, wild fires and prescribed burning. In addition to individual profiles, composite profiles are also important for SPECIATE users. The journal article "An assessment of important SPECIATE profiles in the EPA emissions modeling platform and current data gaps" (Bray, et. al., 2019) provides further details on profile needs. A few improvements stemming from this work were made to the SPECIATE database: an AE6 version of a forest fires profile was added, and an updated set of consumer products profiles were added.

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 5.0 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 5.0 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 VINTAGE 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 5.0 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 a group of compounds never has both identifiers. Finally, ongoing research and analysis shows that there are compounds and mixtures that have no associated identification numbers.

Within the SPECIATE 5.0 database, all species, whether individual compounds or groupings, are identified and detailed in the SPECIES_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 5.0 database, rather than a particular ID number (such as CAS or EPA ID). Thus, the SPECIATE 5.0 database can function with or without the presence of a CAS or EPA ID.

The SPECIES_ID field in the SPECIES_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 SRS ID is subsequently defined for a compound or group, that information will be recorded in the SPECIATE database in the SPECIES_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 5.0 database in the SPECIES_PROPERTIES table.

Storage and retrieval of aerometric data (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 SWG is undecided about whether they should be included in the SPECIATE database. For SPECIATE 5.0, the SAROAD codes associated with SPECIATE 3.2 profiles are kept in the database.

Additional species properties were added in SPECIATE 5.0 related to the volatility (i.e. vapor pressure) and oxygen content (i.e. oxygen to carbon ratio) of explicit compounds and lumped groups of compounds.

Two vapor pressure fields, both in units of Pascal, were added in the SPECIES_PROPERTIES table. Two methods (and hence two fields) were used: 1) VP_Pascal_EPI, from the EPISUITE model (recommended by Ben Murphy, EPA/ORD) and, 2) UMANSYSPROP tool.

E. Mass Fractions of Unmeasured Species

To account for as much as possible of the emitted mass of $PM_{2.5}$, 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, nonroad gasoline exhaust, onroad 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

Species	Oxide Form 1	Oxide Form 2	Oxide Form 3	Oxygen/Metal Ratio
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 PM. 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 SWG assumed all K to be in the form of KCl rather than K_2O.

In SPECIATE 5.0, the SWG revised the approach for computing MO. For Mg, Na, Ca and K, rather than use the oxygen/metal ratio applied to the weight percent of ionic or atomic forms, the SWG decided that it should be applied to the difference between the atom and the ion (e.g., K – K+) and if there were not both forms, then contribution to total MO from that species is set to 0. The reason we did this is because the oxygen would not bind with the ionic form and we did not want to overestimate the MO so we chose to

use only the difference between the atomic and ionic form, or 0 if the data for both ionic and atomic form were not available.

Particulate Non-Carbon Organic Matter (PNCOM)

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 OM/OC ratio to calculate an OM emission, and subtracting OC from OM. For all new profiles added to SPECIATE 4.5 after 2016, we used the methods described in Reff et al. (2009) unless PNCOM was explicitly measured and reported in the source tests or if a different value was assumed in the reference providing the data for the profile.

Reff et al. (2009) used an OM/OC ratio of 1.25 for all motor vehicle exhaust sources (LDDV and HDDV exhaust, nonroad and onroad 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). Some mobile source profiles created by EPA after the Reff paper (e.g., from the Kansas City Study and documented in EPA, 2018a) use a factor of 1.2.

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 × [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 × [Al] + 2.49 × [Si] + 1.63 × [Ca] + 2.42 × [Fe] + 1.94 × [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.

In SPECIATE 5.0, the procedures were slightly modified, with respect to the calculation of MO for associated with certain metals. The revised protocol is provided in Appendix G.

G. Avoiding Double-Counting Compounds

The total speciated percentage of a given PM profile is listed under the TOTAL field in the SPECIATE 5.0 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 flame atomic absorption or ion chromatography analysis are used, since these techniques provide a higher total mass than the elemental measurements. The SWG also adopts DRI's protocol for including the following compounds in the total speciated percentage calculation. The included compounds are ammonium, chlorine atom, nitrate, phosphorus, potassium, and sodium ion. To avoid double counting, the excluded compounds are ammonia, chloride ion, phosphate, potassium ion, and sodium atom.

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 PM profile (field called "TOTAL"). The SWG 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 (INCLUDES_INORGANIC 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 5.0 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 5.0. The terms "adjusted for oxygenates" and "not adjusted for oxygenates" are added to the end of the names of the profiles in the PROFILES table in the SPECIATE 5.0 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 5.0 database includes an analytical methods field (ANALYTICAL METHOD) in the SPECIES table indicating which method is used.

K. AE6 and Volatility Basis Set (VBS) Profiles

Several profile types in SPECIATE are included to support compatibility with photochemical air quality models such as CMAQ. These are typically profiles for which the raw measurement data are aggregated and/or non-measured species are derived from the measured species. These profile types are: PM-Simplified, PM-AE6, PM-VBS and VOC-VBS.

PM-AE6 profiles have been included in SPECIATE since SPECIATE 4.3. These were added to support PM speciation compatibility with the AE6 aerosol module in the CMAQ photochemical model (versions 5.0 and later). This model requires emissions of PNCOM, particulate-bound water, ammonium, sodium, chloride and 8 trace metals as distinct model species using the approach in Reff et al. (2009). These are discussed in more detail in Appendix G.

To provide additional metadata on these AE6 profiles the following fields were added to SPECIATE 5.0:

- ORGANIC_MATTER_to_ORGANIC_CARBON_RATIO – this is the factor used to convert primary organic carbon (POC) to PNCOM which is required for AE6 profiles
- MASS_OVERAGE_PERCENT – this is the percentage of mass over 100% prior to adjustment of the profile to no more than 101% (required for AE6)

SPECIATE 5.0 is the first version that includes profiles to support the VBS of CMAQ5.3. To do this, EPA added numerous fields to SPECIATE and a few SPECIATE PM-VBS and GAS-VBS profiles. The VBS serves to better characterize semi-volatile compounds in gas and PM profiles.

Additional fields were added to the PROFILES table and SPECIES_PROPERTIES table as directed. These additional fields help to determine proper partitioning of the organic mass in the profile between gas and particle phase and further document the conditions under which the measurement study was done.

Fields added to the PROFILES table to help support VBS are:

- TEMP_SAMPLE_C
- RH_SAMPLE
- PARTICLE_LOADING_ug_per_m3
- ORGANIC_LOADING_ug_per_m3

The following fields were added to the SPECIES PROPERTIES table:

- VP_ PASCAL_UM
- VP_Pascal_EPI
- OC_to_OM ratio

These enable users to assign specific species measured to the proper VBS species. While not added for SPECIATE 5.0, we will consider adding the Oxygen to Carbon ratio at the profile level for a subsequent SPECIATE version.

In addition, 20 VBS species were added to the SPECIES_PROPERTIES table which are based on the saturation concentration (C*). These species and selected SPECIES_PROPERTIES fields are provided in Table 6.

Table 6. New Species added to SPECIATE 5.0 for VBS

ID	NAME	SYMBOL	NOTE	O_to_C_ RATIO	VP_ Pascal_ EPI
3254	PNCOMN2, C* = 1e-2 ug m-3	PNCOMN2	Primary Organic Non-Carbon Mass of Saturation Concentration (C*) 0.01 ug m-3 measured in the particle phase		
3253	PNCOMN1, C* = 1e-1 ug m-3	PNCOMN1	Primary Organic Non-Carbon Mass of Saturation Concentration (C*) 0.1 ug m-3 measured in the particle phase		
3252	PNCOMP0, C* = 1e0 ug m-3	PNCOM0	Primary Organic Non-Carbon Mass of Saturation Concentration (C*) 1 ug m-3 measured in the particle phase		
3251	PNCOMP1, C* = 1e1 ug m-3	PNCOMP1	Primary Organic Non-Carbon Mass of Saturation Concentration (C*) 10 ug m-3 measured in the particle phase		
3250	PNCOMP2, C* = 1e2 ug m-3	PNCOMP2	Primary Organic Non-Carbon Mass of Saturation Concentration (C*) 100 ug m-3 measured in the particle phase		
3249	POCN2, C* = 1e-2 ug m-3	POCN2	Primary Organic Carbon Mass of Saturation Concentration (C*) 0.01 ug m-3 measured in the particle phase		
3248	POCN1, C* = 1e-1 ug m-3	POCN1	Primary Organic Carbon Mass of Saturation Concentration (C*) 0.1 ug m-3 measured in the particle phase		
3247	POCP0, C* = 1e0 ug m-3	POC0	Primary Organic Carbon Mass of Saturation Concentration (C*) 1 ug m-3 measured in the particle phase		
3246	POCP1, C* = 1e1 ug m-3	POCP1	Primary Organic Carbon Mass of Saturation Concentration (C*) 10 ug m-3 measured in the particle phase		
3245	POCP2, C* = 1e2 ug m-3	POCP2	Primary Organic Carbon Mass of Saturation Concentration (C*) 100 ug m-3 measured in the particle phase		
3244	Aromatic IVOCP5, C* = 1e5 ug m-3	IVOCP5ARO	Intermediate Volatility Aromatic Organic Compounds of Saturation Concentration (C*) 100,000 ug m-3, C13. MW is an average of single-ring aromatic and PAH species with C* = 10^5 ug m-3 detected in mobile source vehicle NMOG emissions		1.530135
3243	Aromatic IVOCP6, C* = 1e6 ug m-3	IVOCP6ARO	Intermediate Volatility Aromatic Organic Compounds of Saturation Concentration (C*) 1,000,000 ug m-3, C15.5. MW is an average of single-ring aromatic and PAH species with C* = 10^6 ug m-3 detected in mobile source vehicle NMOG emissions.		12.58284
3242	SVOCN1, C* = 1e-1 ug m-3	SVOCN1	Semi-volatile Organic Compounds of Saturation Concentration (C*) 0.1 ug m-3. MW based on assignment to representative alkane,C34.5		5.100451E-07
3241	SVOCP0, C* = 1e0 ug m-3	SVOCP0	Semi-volatile Organic Compounds of Saturation Concentration (C*) 1 ug m-3. MW based on assignment to representative alkane,C31		5.672355E-06
3240	SVOCP1, C* = 1e1 ug m-3	SVOCP1	Semi-volatile Organic Compounds of Saturation Concentration (C*) 10 ug m-3. MW based on assignment to representative alkane,C27.5		6.388709E-05
3239	SVOCP2, C* = 1e2 ug m-3	SVOCP2	Semi-volatile Organic Compounds of Saturation Concentration (C*) 100 ug m-3. MW based on assignment to representative alkane,C24		7.312151E-04
3238	IVOCP3, C* = 1e3 ug m-3	IVOCP3	Intermediate Volatility Organic Compounds of Saturation Concentration (C*) 1,000 ug m-3. MW based on assignment to representative alkane,C21		8.346193E-03
3237	IVOCP4, C* = 1e4 ug m-3	IVOCP4	Intermediate Volatility Organic Compounds of Saturation Concentration (C*) 10,000 ug m-3. MW based on assignment to representative alkane,C18		9.720859E-02
3236	IVOCP5, C* = 1e5 ug m-3	IVOCP5	Intermediate Volatility Organic Compounds of Saturation Concentration (C*) 100,000 ug m-3. MW based on assignment to representative alkane,C15.5		1.126736
3235	IVOCP6, C* = 1e6 ug m-3	IVOCP6	Intermediate Volatility Organic Compounds of Saturation Concentration (C*) 1,000,000 ug m-3. MW based on assignment to representative alkane, C13		13.47184

With the release of SPECIATE 5.0, we have introduced profiles for mobile sources (vehicles, offroad mobile, and aircraft) that explicitly distribute organic mass among low volatility, semi-volatile, intermediate volatility and volatile organic compounds (LVOCs, SVOCs, IVOCs, and VOCs, respectively). These were developed from data from both existing and new measurement studies as presented in Lu et al., 2018. The profiles have been shown to be highly consistent with existing mobile profiles in the VOC range. However, much of the IVOC and SVOC mass has been underrepresented in the past. The new profiles offer a more complete picture of emissions in these ranges, and the resulting secondary organic aerosol (SOA) formation that follows. To accommodate these important classes of pollutants, we use the new species added to the SPECIATE database, with properties chosen to effectively propagate information about the partitioning behavior of emissions from individual sources to downstream models, including large-scale 3D models. Unlike AE6 profiles, the mass can exceed 100% for the PM-VBS profiles because the estimate is now accounting for the total mass of SVOCs, some of which may have been undetected by particle emission measurement techniques.

The workbook developed for these profiles shows the calculations used to transform PM-AE6 into VBS and provides the data for the GAS-VBS profiles. For these initial profiles the new metadata fields added to the PROFILE table were not available, but the SWG thought it was necessary to include them to indicate to researchers the additional measurements that are needed to inform the model developers as they advance the incorporation of VBS in the atmospheric models

L. Data from Tunnel Studies

No profiles from tunnel studies were added to SPECIATE 5.0, however, they are in the database from previous versions. 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. In some cases, where certain lanes of the tunnel are restricted to onroad light-duty or onroad heavy-duty vehicles, the profile could be identified as an onroad gasoline or onroad diesel profile, respectively. In addition, emissions measured in these studies may only represent limited modes of operation under certain conditions (e.g vehicles traveling at relatively constant speed).

M. TOG-to-VOC RATIO

The process of calculating the TOG-to-VOC RATIO (previously called VOC-to-TOG conversion factor in SPECIATE 4.5 and older versions) for a given profile consists of determining the species in the profile that are exempted from the EPA's regulatory definition of VOC. The formula is provided in Table 1. The EPA's regulatory definition of VOC and the updated list of exempt VOC are available in the Electronic Code of Federal Regulations: Title 40 → Chapter I → Subchapter C → Part 51 → Subpart F → §51.100. A direct link is here: http://www.ecfr.gov/cgi-bin/text-idx?SID=b77fd17146a534c225c8557b5ed4a469&node=40:2.0.1.1.2.3.8.1&rgn=div8 (*last accessed March 2019*).

Based on the EPA's list of exempt VOCs, database queries are used to compute the TOG-to-VOC RATIO. For example, if a profile contains 20% methane (an exempt VOC) and 80% VOC, the TOG-to-VOC RATIO 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.

N. Composite PM and TOG Profiles

Many emission source categories have multiple speciation profiles in prior SPECIATE versions. All profiles from prior SPECIATE versions are carried forward to SPECIATE 5.0. There are 131 composite PM profiles (Reff et al., 2009) carried forward into the SPECIATE 5.0 database. There are four composite tire dust and brake wear PM profiles (95495 – 95462) added to SPECIATE 4.5 and carried forward into the SPECIATE 5.0 database. Additional composite profiles were added to SPECIATE 5.0. Users may utilize composite profiles to avoid manual comparison of several relevant, but diverse, profiles as they were created by the SWG to be representative of the average 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 CODE that start with "91xxx." The term "composite" is also included at the end of the name in the NAME field in the PROFILES table. The composite profiles are easily identified by the ORIGINAL_COMPOSITE field (allowed value = "O" for Original, "C" for Composite, Null for legacy profiles). The PROFILE_NOTES field in the PROFILES 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 KEYWORD_REFERENCE table; the REF_DOCUMENT field in the KEYWORD_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 ones supporting the PM-composite profiles. 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. In these 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 5.0. 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 codes 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 (EFs) for prescribed burning and wildfires in United States (Urbanski, 2014).

O. Molecular Weights

The SPECIATE 5.0 database contains a SPECIES_PROPERTIES table that includes 2,814 unique species (both individual compounds and mixtures). Since SPECIATE 5.0 includes all profiles from SPECIATE 3.2, the molecular weights (MWs) as well as other species information are included in the SPECIATE 5.0 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 MW from the same class of compounds is applied. For example, Species ID 2624 (1,4-Dimethyl-2-ethylcyclohexane), the MW 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.

P. 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 5.0 to document changes in quality assurance/quality control responsibilities and refinements to procedures. This document is available by request.

Q. 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 SWG continues to add new source profiles and improve the functions and quality of the database, the SWG 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 SWG recommends not changing or removing any numbers from previously published SPECIATE versions. The SWG'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 codes is added in the NOTES field in the PROFILES table;
2. The note is then documented in the REVISION_LIST table that records all changes made to the database; and
3. The corrected profile is added to the database and assigned the original profile code, e.g., profile code 4567, with an alpha notation like 4567a and further refinements with b, c, d, and so on.

Note that the above convention was not always done with SPECIATE profiles so reading the notes remains important.

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, EF 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 EFs (e.g., mg/kilogram of biomass burned, mg/kilometer traveled, and mg/kilogram of meat cooked). For each source type, EFs of all speciated compounds and unidentified species (when available) are summed to obtain the total VOC or TOG EFs. The individual species EFs are then divided by the total EFs 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 MW (30.07)] ÷ [2 × carbon MW (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 U. S. (e.g., from sources such as chemfinder.com). These chemical names are consistent with those available in the EPA SRS database (https://iaspub.epa.gov/sor_internet/registry/substreg/searchandretrieve/substancesearch/search.do (*last accessed April 2019*). 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 5.0 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 SWG 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 (VINTAGE RATING) and number of samples (DATA QUANTITY RATING). For example, Profile codes 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.

   The SWG developed a quality assessment scoring system (QSCORE, see Appendix E) to easily recognize and assign value points to indicators of a strong, well planned and executed study, which is presented in a complete and logical manner. The comprehensive evaluation framework guides the reviewer to assign quality value points to the areas of the study deemed most important for use in SPECIATE. Therefore, SPECIATE users are encouraged to consider QSCORE, which is only available for new profiles in SPECIATE 5.0, over profile quality ratings.

CHAPTER VI. Future Directions

This section outlines future work we see as being needed to improve SPECIATE. Some of this work has been started with SPECIATE 5.0 and needs to be further thought out and extended. Other parts have not yet begun but should be considered moving forward.

- **Interim Releases of SPECIATE**: Currently we have an approximately triennial process to update the SPECIATE database and make it available to the general public. This future work will focus on development of interim releases to make profiles available before triennial major releases of SPECIATE. This would allow for improvements in both modeling and assessments based on these updated interim profiles. The rigor of getting these profiles into SPECIATE, even with an interim release, would remain the same as described earlier in this document. For example, we already have a number of data sources on SPECIATE's Master Evaluation of Profiles spreadsheet (from which we can develop new SPECIATE profiles). In addition, EPA's ORD is conducting testing of sources of interest such as biomass burning, data from which profiles can be updated more timely with interim releases.
- **Streamline Data Entry into SPECIATE**: The SWG is interested to explore more streamlined ways to add data into SPECIATE. This could include new software or techniques for getting the requisite data for a source-testing program into SPECIATE. This may also allow for team members to more easily accomplish this task and added quality assurance to ensure the proper species information (names, synonyms) are entered. Ideally the process can be expanded to the broader community so that those collecting the data can provide them directly into SPECIATE.
- **Identify Profiles used in Air Quality Modeling**: There are sometimes requests for a list of profiles that are used in photochemical air quality regulatory modeling, that information is not easily available currently in SPECIATE. Future work would include development of a tool that will enable users to explore the profiles that are being used/have been used in different modeling platforms, further allowing for downloading that information into a convenient format such as Microsoft Excel®.
- **Including Volatility Basis Set (VBS) fields in SPECIATE**: VBS provides a unified framework for gas-aerosol partitioning of low volatility particle-phase compounds, semi-volatile compounds, and VOCs. A better characterization of such a set of compounds begins with better and more complete information being contained in SPECIATE for both PM and VOC composition. Recent studies have revealed that POA, SOA, and the organic vapors in equilibrium with them, together form a dynamic system that constantly evolves due to multi-generation oxidation. First, POA, previously treated as nonvolatile and nonreactive, can evaporate, oxidize, and re-condense to form SOA, which is known as aging of POA. Second, gas-phase oxidation products of traditional SOA precursors (i.e., NMHCs) can undergo multiple generations of oxidation, which has been demonstrated by smog-chamber experiments using gas-phase oxidation products as reactants (Ng et al., 2011; Lambe et al., 2012; Tkacik et al., 2014). Third, IVOCs, currently not included or misclassified in emission inventories, have been shown to make a substantial contribution to the SOA budget in spite of being a small fraction of the overall organic gas emissions for many sources like gasoline vehicles (Robinson et al., 2007; Zhao et al., 2014; Lu et al., 2018). All of these new processes could lead to elevated SOA levels and oxidation state, but they are not accounted for in most chemical transport models (CTMs); inclusion can help explain the differences between model predictions and measurements. To address this in SPECIATE, we have begun to include fields that can hold the type of information needed by air quality modelers to access these data for more robust modeling. As discussed Chapter IV (Section K), we also added a small number of PM-VBS and Gas-VBS profiles to SPECIATE 5.0. However, this work in SPECIATE is in its infancy. The goal moving forward would be to better understand PM and VOC test results, make sure researchers are measuring what we need so that we have better-

resolved lumped categories based on the most recent methods of detection and adding single-compounds where we have information on them.

As we move forward, for POC, we should recognize that users are interested in moving from the OC/NCOM paradigm we have now to something more compound focused (total OM from single compounds or classes of compounds), consistent with how we handle the VOC side currently. This shift in focus will impact how speciation measurements are made and assist in how CTMs use the organic mass. Results to date suggest that the partitioning of OC mass does not respond to OC; it responds to OM. Total OM is therefore, for modeling efforts, more important to constrain than OC, although both are important. The proposal suggests we continue to provide the OC as a diagnostic species in every profile -- this is useful information, particularly because it exists for so many sources now. But as we move forward, we should strive to provide the profiles with compounds or classes in terms of their total OM and discontinue downstream use of the OC and NCOM altogether when possible. This would mean that SPECIATE would need to accommodate such test results and that a redesign is needed for software that processes profiles so they may be used in CTMs.

- **Make more complete inclusion of actual EFs in SPECIATE**: The main focus on SPECIATE has been the collection of mass fractions (weight percents). However, these data may have been computed from EFs. In SPECIATE 4.5, the "Other Gases" table had a field for the EF, but the Gas and PM tables did not. In SPECIATE 5.0, these tables are combined, resulting in a field for the species EF. We also added a field for the master pollutant (e.g., TOG, PM) EF. We have populated a small number of the profiles with actual EFs as available from research studies. In the future, we should continue to add data as we have it for all the more recent profiles in SPECIATE. Having EFs would help bridge the potential mis-match that occurs when fractions measured at vastly different conditions are married with master pollutants (VOC or PM) which could have been measured at not only different conditions but also with totally different test methods.
- **Improve Speciation Tool**: The Speciation Tool uses SPECIATE data as a key input in order to create model-ready profiles from the "raw" species profiles in SPECIATE. The tool creates TOG profiles for numerous photochemical mechanisms. For PM profiles, some calculations and manipulation of the measured data needs to be done in SPECIATE in order for the Speciation Tool to create the model-ready profiles for the air quality modeling. Work on including the capability for developing PM-AE6 ready profiles into the Speciation Tool would alleviate the need to put model-ready profiles into SPECIATE. This may require additional metadata for SPECIATE. For example, an important step is to reconstruct the PM mass and to make adjustments if the sum of reconstructed species weight percents exceeds 100%. Since a profile may include species that would double count mass if summed together, it would be important to indicate which species in the PM profile would double count one another (e.g., a PM profile with specific individual polycyclic aromatic hydrocarbons would double count POC and PNCOM).
- **Follow up on SPECIATE needs:** As discussed in Chapter IV, Section A, we have identified profiles that need updates or new data. To follow up on this study, we first would explore the data in SPECIATE to determine whether any existing profiles are available in the database that would address the needs. The next step would be to conduct a literature search and outreach to the research community to seek new data.
- **Improved Outreach of SPECIATE needs and availability**: Better outreach to researchers, both internal and external, on what's needed beyond just the mass fractions, including some of the new needs identified earlier in this section and needs for more complete metadata.

References

Allen, 2004: Allen, D., University of Texas at Austin, e-mail communication with the SPECIATE Workgroup, August 8, 2004.

Beck, 2004: Beck, L., U.S. EPA, personal communication (internal data collection effort) with Ying Hsu, E.H. Pechan & Associates, Inc., 2004.

Brantley et al., 2015, Brantley, H. L., Thoma, E. D., and Eisele A. P., Assessment of VOC and HAP Emissions from Oil and Natural Gas Well Pads Using Mobile Remote and Onsite Direct Measurements, Journal of the Air & Waste Management Association, DOI: 10.1080/10962247.

Bray et al., 2017, Bray, C.D. Strum, M. Simon, H. Riddick, L. Kosusko, M., Rao, V., Assessment of Important SPECIATE Profiles on EPA's Emissions Modeling Platform, Presentation at 2017 International Emission Inventory Conference, "Applying Science and Streamlining Processes to Improve Inventories," RTP, NC, August 15, 2017. https://www.epa.gov/sites/production/files/2017-11/documents/speciate_profiles.pdf (*last accessed April 2019.*

Bray et. al., 2019, Bray, C.D., Strum, M., Simon, H. Riddick, L. Kosusko, M., Menetrez, M., Hays, M.D., Rao, V., An Assessment of Important SPECIATE Profiles in the EPA Emissions Modeling Platform and Current Data Gaps, Atmospheric Environment, In Press. DOI: 10.1016/j.atmosenv.2019.03.013

Cantu, 2003: Cantu, G., Speciation of Texas Point Source VOC Emissions for Ambient Air Quality Modeling,

Texas Commission on Environmental Quality, 2003, http://www.tceq.texas.gov/assets/public/implementation/air/rules/stakeholder/hrvoc/2004-02-06/voc-speciation-report.pdf (*last accessed April 2019*.

CARB, 1991: Censullo, A.C., Development of Species Profiles for Selected Organic Emission Sources, California Polytechnic State University, California Air Resources Board Contract A832-059, April 30, 1991.

CARB, 2018: Speciation Profiles Used in ARB Modeling, California Air Resources Board, http://www.arb.ca.gov/ei/speciate/speciate.htm (*last accessed April 2019*.

Carter, 2004: Carter, W., University of California at Riverside, personal communication with Ying Hsu, E.H. Pechan & Associates, Inc., June 23, 2004.

Chow et al., 1999: Chow, J.C., Watson, J.G., Green, M.C., Lowenthal, D.H., DuBois, D.W., Kohl, S.D., Egami, R.T., Gillies, J.A., Rogers, C.F., Frazier, C.A., Cates, W., Middle- and Neighborhood-Scale Variations of PM_{10} Source Contributions in Las Vegas, Nevada, *Journal of the Air & Waste Management Association*, 49: 641-654, 1999.

Chow, 2004: Chow, J.C., Desert Research Institute, personal communication with the SPECIATE Workgroup, August 18, 2004.

CRC, 2003: Gautam, M. et al., Heavy-Duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory, Phase I, prepared by West Virginia University Research Corporation for the Coordinating Research Council, Inc., CRC E-55/59, 2003, http://www.crcao.org/reports/recentstudies2003/E-7a%20reports/E-55-59%20Phase%20I%20Report.pdf (*last accessed April 2019*.

CRC, 2005: Gautam, M. et al., Heavy-Duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory, Phase II, prepared by West Virginia University Research Corporation for the Coordinating Research Council, Inc., CRC E-55/59-2, 2005.

CRC, 2007: Gautam, M. et al., Heavy-Duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory, Final Report, CRC E-55/59, prepared by West Virginia University Research Corporation for the Coordinating Research Council, Inc., 2007, http://www.crcao.com/reports/recentstudies2007/E-55-59/E-55_59_Final_Report_23AUG2007.pdf (*last accessed April 2019*)

CRC, 2011: Coordinating Research Council, Inc., Exhaust and Evaporative Emissions Testing of Flexible-Fuel Vehicles, CRC Report CRC-E-80, August 2011, http://www.crcao.org/publications/emissions/index.html (*last accessed April 2019*)

DOE, 2005: Gasoline/Diesel PM Split Study: Source and Ambient Sampling, Chemical Analysis, and Apportionment Phase, Draft Final Report, prepared by E.M. Fujita, B. Zielinska, W.P. Arnott, D.E. Campbell, L. Reinhart, J.C. Sagebiel and J.C. Chow, Desert Research Institute for the National Renewable Energy Laboratory, September 30, 2005, NREL Subcontract Nos. ACL-1-31046-01 and ACL-1-31046-02.

Eklund et al., 1998: Eklund, B., Anderson, E.P., Walker, B.L., and Burrows, D.B., Characterization of Landfill Gas Composition at the Fresh Kills Municipal Solid-Waste Landfill, *Environmental Science and Technology*, 32: 2233-2237, 1998.

EPA, 1984: Bennett, R.L., Knapp, K.T., Duke, D.L., 1984. Chemical and Physical Characterization of Municipal Sludge Incinerator Emissions, U.S. Environmental Protection Agency, Research Triangle Park, NC. EPA-600/S3-84-047.

EPA, Work Assignment WA 2-02 – Emissions Modeling Platform Support, Personal communication with U.S. Environmental Protection Agency Alexis Zubrow of Office of Air Quality Planning and Standards.

EPA, 2003: Source Sampling Fine Particulate Matter: A Kraft Process Recovery Boiler at a Pulp and Paper Facility, Volumes I and II, prepared by Eastern Research Group, Inc. for Air Pollution Prevention and Control Division, National Risk Management and Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency. EPA-600/R-03/099a, 2003.

EPA, 2008a: Nam, E., Fulper, C., Warila, J, Somers, J., Michaels, H., Baldauf, R., Rykowski, R., and Scarbro, C., Analysis of Particulate Matter Emissions from Light-Duty Gasoline Vehicles in Kansas City, Office of Transportation and Air Quality and Office of Research and Development, U.S. Environmental Protection Agency, EPA420-R-08-010, 2008.

EPA, 2008b: Kansas City PM Characterization Study, Office of Transportation and Air Quality, U.S. Environmental Protection Agency, EPA420-R-08-009, 2008.

EPA, 2009: Exhaust Emission Profiles for EPA SPECIATE Database: Energy Policy Act (EPAct) Low-Level Ethanol Fuel Blends and Tier 2 Light-Duty Vehicles, Office of Transportation and Air Quality, U.S. Environmental Protection Agency, EPA-420-R-09-002, 2009.

EPA, 2010: Hydrocarbon Composition of Gasoline Vapor Emissions from Enclosed Fuel Tanks, Office of Transportation and Air Quality and Office of Research and Development, U.S. Environmental Protection Agency, EPA-420-D-10-001, 2010.

EPA, 2011a: Composition of Natural Gas for use in the Oil and Natural Gas Sector Rulemaking, memorandum from EC/R to Bruce Moore, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, on July 28, 2011, EPA-HQ-OAR-2010-0505, http://www.regulations.gov/#!documentDetail;D=EPA-HQ-OAR-2010-0505-0084 (*last accessed April 2019)*

EPA, 2011b: Hydrocarbon Composition of Gasoline Vapor Emissions from Enclosed Fuel Tanks, Office of Transportation and Air Quality and Office of Research and Development, U.S. Environmental Protection Agency, EPA-420-R-11-018, 2011.

EPA, 2015a: Tribal Minor Source Registration Data - Uintah & Ouray Indian Reservation, sent by Cindy Beeler of U.S. Environmental Protection Agency Region 8, Energy Advisor, Office of the Regional Administrator on 8/10/2015.

EPA, 2015b: Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES 2014, U.S. Environmental Protection Agency, EPA-420-R-15-022, November 2015

EPA, 2015c: Speciation Profiles and Toxic Emission Factors for Nonroad Engines, U.S. Environmental Protection Agency, EPA-420-R-14-028, Appendix A, March 2015.

EPA, 2016. 2014 national emissions inventory (NEI) data. https://www.epa.gov/air-emissions-inventories/2014-national-emissions-inventory-nei-data (*last accessed April 2019*)

EPA, 2018a. 2014-2016 version 7 air emissions modeling platforms. https://www.epa.gov/air-emissions-modeling/2014-2016-version-7-air-emissions-modeling-platforms (*last accessed April 2019*)

EPA, 2018b: Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014b, EPA-420-R-18-012, July 2018.

ERG, 2001: Source Sampling Fine Particulate Matter: Wood-fired Industrial Boiler, prepared by Eastern Research Group, Inc for Air Pollution Prevention and Control Division, U.S. Environmental Protection Agency, EPA-600/R-01-106, 2001.

ERMD Report 00-37: Graham, L. and Welburn C., Gaseous and Particulate Matter Emissions from Two In-Use Urban Transit Buses - Tested in 20 ºC and -10 ºC, Emissions Research and Measurement Division, Environment Canada, 2000.

ERMD Report 05-39: Belisle, S., and Graham, L., Comparison of Emissions of Conventional and Flexible Fuel Vehicles Operating on Gasoline and E85 Fuels, Emissions Research and Measurement Division, Environment Canada, 2005.

ERMD Report 98-26718: Graham, L., Howes, P., and Rideout, G., Investigation of Potential Exhaust Emissions Reductions using Biodiesel Blends in a Conventional Diesel Engine, Emissions Research and Measurement Division, Environment Canada,1998.

ERMD 2000-01: Characterization of Organic Compounds from Selected Residential Wood Stoves and Fuels, December 2000.

Gabele, 1997: Gabele, P., Exhaust Emissions from Four-Stroke Lawn Mower Engines, *Journal of the Air & Waste Management Association*, 47: 945-952, 1997.

Gentner et al., 2013, Gentner, D. R., Worton, D. R., Isaacman, G., Davis, L. C., Dallmann, T. R., Wood, E. C., Herndon, S. C., Goldstein, A. H., and Harley, R. A., Chemical Composition of Gas-Phase

Organic Carbon Emissions from Motor Vehicles and Implications for Ozone Production, *Environmental Science and Technology*, 47: 11837–11848, 2013.

Hays et al., 2002: Hays, M.D., Geron, C.D., Linna, K.J., Smith, N.D., Schauer, J.J., Speciation of Gas-Phase and Fine Particle Emissions from Burning of Foliar Fuels, *Environmental Science and Technology*, 36: 2281-2295, 2002.

Hays et al., 2005: Hays, M.D., Fine, P.M., Geron, C.D., Kleeman, M.J., and Gullett, B.K, Open Burning of Agricultural Biomass: Physical and Chemical Properties of Particle-Phase Emissions, *Atmospheric Environment*, 39: 6747-6764, 2005.

Hays et al., 2008: Hays, M.D., Beck, L., Barfield, P., Lavrich, R.J., Dong, Y, and VanderWal, R.L., Physical and Chemical Characterization of Residential Oil Boiler Emissions, *Environmental Science and Technology*, 42: 2496–2502, 2008.

Hays et al., 2011: Hays, M. D., Gullett, B., King, C., Robinson, J., Preston, W. and Touati, A., Characterization of Carbonaceous Aerosols Emitted from Outdoor Wood Boilers, *Energy Fuels*, 25: 5632–5638, 2011.

Hays et al., 2013: Carbonaceous Aerosols Emitted from Light-Duty Vehicles Operating on Gasoline and Ethanol Fuel Blends, *Environmental Science and Technology,* 47:14502–14509, 2013

Health Effects Institute, Research Report 133. Characterization of Metals Emitted from Motor Vehicles by Schauer et al., 2006.

Herrington et al., 2012: Herrington, J.S., Hays, M.D., George, B.J., and Baldauf, R.W. The Effects of Operating Conditions on Semivolatile Organic Compounds Emitted from Light-Duty Gasoline-Powered Motor Vehicles, *Atmospheric Environment*, 54: 53-59, 2012.

Howard et al., 2010, Howard, C. J., Kumar, A., Mitloehner, F., Stackhouse, K., Green, P. G., Flocchini, R. G., and Kleeman, M. J., Direct Measurements of the Ozone Formation Potential from Livestock and Poultry Waste Emissions, *Environmental Science and Technology,* 44, 2292–2298, 2014.

Hsu, 2003: Hsu, Y., Methodology for Speciation of Organic Gas Hot Soak Emissions –California Light-Duty Vehicles, California Air Resources Board, July 23, 2003. http://www.arb.ca.gov/ei/speciate/hotsoakspemeth.pdf (*last accessed April 2019*)

Hsu and Mullen, 2007: Hsu, Y., and Mullen, M., Compilation of Diesel Emissions Speciation Data, E.H. Pechan & Associates, Inc. for CRC, E-75 and NREL, ES05-03, October 2007, http://www.crcao.com/reports/recentstudies2008/E-75/CRC_E75_Final%20Report_v3.pdf (*last accessed April 2019*)

Huffman et al., 2000: Huffman, G. P., Huggins, F. E., Shah, N., Huggins, R., Linak, W.P., Miller, C.A., Pugmire, R.J., Meuzelaar, H.L.C., Seehra, M.S., and Manivannan, A., Characterization of Fine Particulate Matter Produced by Combustion of Residual Fuel Oil, *Journal of the Air & Waste Management Association*, 50: 1106-1114, 2000.

Japar et al., 1984: Japar, S.M., Szkarlat, A.C., Gorse, Jr., R.A., Heyerdahl, E.K., Johnson, R.L., Rau, J.A., and Huntzicker, J.J., Comparison of Solvent Extraction and Thermal Optical Carbon Analysis Methods: Application to Diesel Vehicle Exhaust Aerosol, *Environmental Science and Technology*, 18: 231-234, 1984.

Jorgensen et al., 1990: Jorgensen, A. D., Picel, K.C., and Stamoudis, V.C., Prediction of Gas Chromatography Flame Ionization Detector Response Factors from Molecular Structure, *Analytical Chemistry*, 62: 683-689, 1990.

Kinsey et al., 2004: Kinsey, J., Linna, K.J., Squier, W.C., Muleski, G.E., and Cowherd, C., Fugitive Particulate Emissions from Construction Mud/Dirt Carryout, *Journal of the Air & Waste Management Association*, 54: 1394–1404, 2004.

Kinsey et al., 2011: Kinsey, J.S., Hays, M.D., Dong, Y., Williams, D.C., and Logan, R., Chemical Characterization of the Fine Particle Emissions from Commercial Aircraft Engines during the Aircraft Particle Emissions eXperiment (APEX) 1 to 3, *Environmental Science and Technology*, 45: 3415–3421, 2011.

Kuhns et al., 2004: Kuhns, H., Chang, M.C., Chow, J.C., Etyemezian, V., Chen, L.W., Nussbaum, N., Nathagoundenpalayam, S., Trimble, D., Kohl, S., MacLaren, M., Abu-Aliban, M., Gillies, J., and Gertler, A., DRI Lake Tahoe Source Characterization Study: Final Report, prepared by DRI for A. Lashgari of California Air Resources Board, October 22, 2004, http://www.arb.ca.gov/research/apr/past/01-734.pdf (*last accessed April 2019*)

Lee et al., 2005: Lee, S., Baumann, K., Schauer, J.J., Sheesley, R. J., Naeher, L. P., Meinardi, S., Blake, D. R., Edgerton, E. S., Russell, A. G., and Clements, M., Gaseous and Particulate Emissions from Prescribed Burning in Georgia, *Environmental Science and Technology,* 39, 9049-9056, 2005.

Lewis, 2004: Lewis, C., U.S. EPA, personal communication (internal data collection effort) with Ying Hsu, E.H. Pechan & Associates, Inc., June 29, 2004.

Liu et al., 2014: Liu, W. T., Chen, S. P., Chang, C. C., Ou-Yang, C. F., Liao, W. C., Su, Y. C., Wu, Y. C., Wang, C. H., and Wang, J. L., Assessment of Carbon Monoxide (CO) Adjusted Non-methane Hydrocarbon (NMHC) Emissions of a Motor Fleet – A Long Tunnel Study, *Atmospheric Environment*, 89, 403 – 414, 2014.

Lambe et al., 2012: Lambe, A. T., Onasch, T.B., Croasdale, D.R., Wright, J. P., Martin, A. T., Franklin, J. P., Massoli, P., Kroll, J. H., Canagaratna, M. R., Brune, W. H., Worsnop, D. R., Davidovits, P., *Environmental Science & Technology* **2012** *46* (10), 5430-5437, DOI: 10.1021/es300274t.

Lu, et al., 2018: Lu, Q., Zhao, Y., and Robinson, A.L., 2018. Comprehensive organic emission profiles for gasoline, diesel and gas-turbine engines including intermediate and semi-volatile organic compound emissions, *Atmospheric Chemistry and Physics*, 18, 17637-17654. http://www.atmos-chem-phys.net/18/17637/2018/ (*last accessed April 2019*)

Machemer, 2004: Machemer, S., Characterization of Airborne and Bulk Particulate from Iron and Steel Manufacturing Facilities, *Environmental Science and Technology*, 38: 381-389, 2004.

McDonald et al. 2003: McDonald, J. D. , Zielinska, B., Fujita, E. M., Sagebiel, J. C., Chow, J. C. and Watson, J. G., Emissions from Charbroiling and Grilling of Chicken and Beef, *Journal of the Air & Waste Management Association*, 53:2, 185-194, DOI: 10.108, 2003.

Ng, et. al. 2011: Ng, N. L., Canagaratna, M. R., Jimenez, J. L., Chhabra, P. S., Seinfeld, J. H., Worsnop, D. R., Changes in organic aerosol composition with aging inferred from aerosol mass spectra, *Atmos. Chem. Phys.*, 11:13,6465-6474, DOI: 10.519 PES 4/acp-11-6465-2011.

Reff and Bhave, 2006: Reff, A. and Bhave, P.V., Emissions Inventory of $PM_{2.5}$ Trace Elements across the U.S., platform presentation given at AAAR International Aerosol Conference, St. Paul, MN, September 2006.

Reff et al., 2009: Reff, A., Bhave, P.V., Simon, H., Pace, T.G., Pouliot, G.A., Mobley, J.D., and Houyoux, M., Emissions Inventory of $PM_{2.5}$ Trace Elements across the United States, *Environmental Science and Technology*, 43: 5790–5796, 2009.

Robinson, et al., 2007. Robinson, A.L., Donahue, N. M., Shrivastava, M., K., Weitcamp, E.A., Sage, A.M., Grieshop, A.P., Lane, T.E., Pierce, J.R., Pandis, S.N., Rethinking of Organic Aerosols: Semivolatile Emissions and Photochemical Aging. *Science*, Vol. 315, Issue 5816, pp. 1259-1262, 2007. DOI: 10.1126/science.1133061.

Rogge et al., 1993: Rogge, W.F., Hildemann, L.M., Mazurek, M.A., Simoneit, B.R.T., and Cass, G.R., Determination of Key Organic Compounds Present in the PM Emissions from Air Pollution Sources, California Air Resource Board Contract Number A932-127, 1993.

Roy et al., Roy, Anirban., Darrell Sonntag, Richard Cook, Catherine Yanca, Charles Schenk, and Yunsoo Choi, Effect of Ambient Temperature on Total Organic Gas Speciation Profiles from Light-Duty Gasoline Vehicle Exhaust, DOI: 10.1021/acs.est.6b01081, *Environ. Sci. Technol.* 2016, 50, 6565−6573

Scanlon, et al., 1985: Scanlon, J.T., and Willis, D.E., Calculation of Flame Ionization Detector Relative Response Factors Using the Effective Carbon Number Concept, *Journal of Chromatography Science*, 23, 333-340, 1985.

Schauer et al., 1998: Schauer, J.J., Kleeman, M.J., Cass, G.R., and Simoneit, B.R.T., Characterization and Control of Organic Compounds Emitted from Air Pollution Sources, California Air Resources Board Contract Number 93-329, 1998.

Schauer et al., 1999: Schauer, J.J., Kleeman, M.J., Cass, G.R, and Simoneit, B.R.T., Measurement of Emissions from Air Pollution Sources. 2. C1 through C30 Organic Compounds from Medium Duty Diesel Trucks, *Environmental Science and Technology*, 33: 1578-1587, 1999.

Shah et. al., 2016: "Composition of Organic Gas Emissions from Flaring Natural Gas," G. Yarwood, T. Shah, Ramboll Environ; A. Eyth and M. Strum, US EPA, Presented at the 2017 International Emission Inventory Conference in Baltimore, MD. https://www.epa.gov/sites/production/files/2017-11/documents/organic_gas.pdf *last accessed April 2019*)

Simon et al., 2010: Simon, H., Beck, L., Bhave, P. V., Divita Jr., F., Hsu, Y., Luecken, D., Mobley, J. D., Pouliot, G. A., Reff, A., Sarwar, G. and Strum, M., The Development and Uses of EPA's SPECIATE Database, *Atmospheric Pollution Research*,1: 196-206, 2010.

Simon et al., 2018: Simon, H., Casey Bray, Madeleine Strum, Heather Simon, Lee Riddick, Mike Kosusko, Marc Menetrez and Venkatesh Rao. "Assessment of important SPECIATE profiles in EPA's emissions modeling platform and current data gaps," 100th Annual AGU Fall Meeting, Washington D.C., December 10-14 2018.

Tkacik et al., 2014: Tkacik, D. S., Lambe, A. T., Jathar, S., Li, X., Presto, A. A., Zhao, Y., Blake, D., Meinardie, S., S., Jayne, J. T., Croteau, P. L., Robinson, *Environmental Science and Technology*, *48* (19), pp 11235–11242, 2014. DOI: 10.1021/es502239v.

TCEQ, 2011, Allen, David T, and Vincent M Torres, University of Texas, Austin. 2011. 'TCEQ 2010 Flare Study Final Report', Texas Commission on Environmental Quality, PGA No. PGA No. 582-8-862-45-FY09-04, Tracking No. 2008-81, Supplemental Support from the Air Quality Research Program, TCEQ Grant No. 582-10-94300.

https://www.tceq.texas.gov/assets/public/implementation/air/rules/Flare/2010flarestudy/2010-flare-study-final-report.pdf (*last accessed April 2019*)

Texas Environmental Research Consortium, 2009, VOC Emissions from Oil and Condensate Storage Tanks, final report prepared by URS Corporation, Comm Engineering, and Trimeric Corporation.

Trabue et al., 2010, Trabue, S., Scoggin, K., Li, H., Burns, R., Xin, H., Hatfield, J., Speciation of Volatile Organic Compounds from Poultry Production, *Atmospheric Environment*, 44, 3538 – 3546, 2010.

U.S. Geological Survey, Professional Paper 1713, Petroleum Systems and Geologic Assessment of Oil and Gas in the San Joaquin Basin Province, California, 2007, http://pubs.usgs.gov/pp/pp1713/(*last accessed April 2019*)

Urbanski, 2014, Urbanski, S., Wildland Fire Emissions, Carbon, and Climate: Emission Factors, *Forest Ecology and Management*, 317, 51–60, 2014.

Woodall et al., 2012: Woodall, B. D., Yamamoto, D.P., Gullett, B. K., and Touati, A., Emissions from Small-Scale Burns of Simulated Deployed U.S. Military Waste, *Environmental Science and Technology*, 46: 10997−11003, 2012.

White and Roberts, 1977: White, W.H., and Roberts, P.T., On the Nature and Origins of Visibility Reducing Aerosols in the Los Angeles Air Basin, *Atmospheric Environment,* 11: 803-812, 1977.

WRAP Phase III Support Data, memo from T. Shah, A. Bar-Ilan, J. Grant, Ramboll Environ. To A. Eyth, R. Mason, A. Zubrow, M. Strum, EPA/OAQPS. "WRAP Phase III oil and gas speciation profiles," 8/27/2015, posted on http://www.wrapair2.org/emissions.aspx (*last accessed April 2019*)

Zhao, et al., 2014: Zhao, Y., Hennigan, C., J., May, A.A., Tkacik, de Gouw, J. A., Gilman, J., B., Kuster, W.C., Borbon, A., Robinson, A.L., *Environmental Science and Technology*, 48 (23), pp 13743–13750, 2014. DOI: 10.1021/es5035188.

APPENDIX A. Listing of New Profiles Added to the SPECIATE 5.0 Database

See Table A-1 on next page.

Table A-1. List of New Organic Gas Profiles (Profile Type = GAS, GAS-VBS) Added to the SPECIATE 5.0 Database

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95476	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Campbell County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Campbell County, Wyoming
95477	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Campbell County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Campbell County, Wyoming
95478	Oil and Gas Production - Composite Profile – Condensate Tank, Campbell County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Condensate Tank, Campbell County, Wyoming
95479	Oil and Gas Production - Composite Profile – Oil Tank, Campbell County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Oil Tank, Campbell County, Wyoming
95480	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Carbon County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Carbon County, Wyoming
95481	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Converse County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Converse County, Wyoming
95482	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Converse County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Converse County, Wyoming
95483	Oil and Gas Production - Composite Profile – Condensate Tank, Converse County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Condensate Tank, Converse County, Wyoming
95484	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Crook County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Crook County, Wyoming
95485	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Fremont County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Fremont County, Wyoming
95486	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Fremont County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Fremont County, Wyoming
95487	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Hot Springs County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Hot Springs County, Wyoming
95488	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Johnson County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Johnson County, Wyoming
95489	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Laramie County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Laramie County, Wyoming
95490	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Lincoln County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Lincoln County, Wyoming
95491	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Lincoln County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Lincoln County, Wyoming
95492	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Niobrara County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Niobrara County, Wyoming
95493	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Sublette County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Sublette County, Wyoming

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95494	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Sublette County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Sublette County, Wyoming
95495	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Sweetwater County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Sweetwater County, Wyoming
95496	Oil and Gas Production - Composite Profile – Condensate Tank, Sweetwater County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Condensate Tank, Sweetwater County, Wyoming
95497	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Sweetwater County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Sweetwater County, Wyoming
95498	Oil and Gas Production - Composite Profile – Raw Gas, Gas Well, Uinta County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Gas Well, Uinta County, Wyoming
95499	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Weston County, Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Weston County, Wyoming
95500	Oil and Gas Production - Composite Profile – Raw Gas, Oil Well, Natrona County Wyoming	GAS	Oil and Gas Production; Composite Profile – Raw Gas, Oil Well, Natrona County, Wyoming
95505	2-stroke Small Off-road Engine Exhaust - MTBE Gasoline	GAS	2-stroke; Small Off-road Engine Exhaust; MTBE Gasoline; leaf blowers; trimmers
95506	4-stroke Small Off-road Engine Exhaust - MTBE Gasoline	GAS	4-stroke; Small Off-road Engine Exhaust; MTBE Gasoline; leaf blowers; trimmers; soil tillers; lawnmowers
95507	Consumer and Commercial Products – Adhesives and Sealants Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; Adhesives and Sealants Composite CARB 2010 Survey
95508	Consumer and Commercial Products – Household Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; Household Composite CARB 2010 Survey
95509	Consumer and Commercial Products – Personal Care Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; Personal Care Composite CARB 2010 Survey
95510	Consumer and Commercial Products – Automotive Aftermarket Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; Automotive Aftermarket Composite CARB 2010 Survey
95511	Consumer and Commercial Products – All FIFRA Related Products Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; All FIFRA Related Products Composite CARB 2010 Survey
95512	Consumer and Commercial Products – Composite CARB 2010 Survey	GAS	Consumer and Commercial Products; Composite CARB 2010 Survey
95513	Architectural Coatings – Solvent and Waterborne Composite CARB 2005 Survey	GAS	Architectural Coatings; Solvent and Waterborne Composite CARB 2005 Survey
95536	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95537	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95538	Oil and Natural Gas Production - Produced Water Pond - Snow covered and icy pond	GAS	Produced water; Oil and gas; Evaporation pond
95539	Oil and Natural Gas Production - Produced Water Pond - Snow covered and icy pond	GAS	Produced water; Oil and gas; Evaporation pond
95540	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95541	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95542	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95543	Oil and Natural Gas Production - Produced Water Pond - Unfrozen netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95544	Oil and Natural Gas Production - Produced Water Pond - Unfrozen netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95545	Oil and Natural Gas Production - Produced Water Pond - partially frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95546	Oil and Natural Gas Production - Produced Water Pond - partially frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95547	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95548	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95549	Oil and Natural Gas Production - Produced Water Pond - Snowy frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95550	Oil and Natural Gas Production - Produced Water Pond - New ice on pond	GAS	Produced water; Oil and gas; Evaporation pond
95551	Oil and Natural Gas Production - Produced Water Pond - New ice on pond	GAS	Produced water; Oil and gas; Evaporation pond
95552	Oil and Natural Gas Production - Produced Water Pond - New ice on pond	GAS	Produced water; Oil and gas; Evaporation pond
95553	Oil and Natural Gas Production - Produced Water Pond - partially frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95554	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95555	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95556	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95557	Oil and Natural Gas Production - Produced Water Pond - Snowy frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95558	Oil and Natural Gas Production - Produced Water Pond - Snowy frozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95559	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95560	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95561	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95562	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95563	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95564	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95565	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95566	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95567	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95568	Oil and Natural Gas Production - Produced Water Pond - Unfrozen briny pond	GAS	Produced water; Oil and gas; Evaporation pond
95569	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95570	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95571	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95572	Oil and Natural Gas Production - Produced Water Pond - Unfrozen pond	GAS	Produced water; Oil and gas; Evaporation pond
95573	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95574	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95575	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95576	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95577	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95578	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95579	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95580	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95581	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95582	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95583	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95584	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95585	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95586	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95588	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95589	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95590	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95591	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95592	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95593	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95594	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95595	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95596	Oil and Natural Gas Production - Produced Water Pond - Netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95597	Oil and Natural Gas Production - Produced Water Pond - Netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95598	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95599	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95600	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95601	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95602	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95603	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95604	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95605	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95606	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95607	Oil and Natural Gas Production - Produced Water Pond - Netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95608	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95609	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95610	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95611	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95612	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95613	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95614	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95615	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95616	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95617	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95618	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95619	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95620	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95621	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95622	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95623	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95624	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95625	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95626	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95627	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95628	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95629	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95630	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95631	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95632	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95633	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95634	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95635	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95636	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95637	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95638	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95639	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95640	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95641	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95642	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95643	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95644	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95645	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95646	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95647	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95648	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95649	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95650	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95651	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95652	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95653	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95654	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95655	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95656	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95657	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95658	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95659	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95660	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95661	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95662	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95663	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95664	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95665	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95666	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95667	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95668	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95669	Oil and Natural Gas Production - Produced Water Pond - Netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95670	Oil and Natural Gas Production - Produced Water Pond - Netted pond	GAS	Produced water; Oil and gas; Evaporation pond
95671	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95672	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95673	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95674	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95675	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95676	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95677	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95678	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95679	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95680	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95681	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95682	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95683	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95684	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95685	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95686	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95687	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95688	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95689	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95690	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95691	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95692	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95693	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95694	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95695	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95696	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95697	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95698	Oil and Natural Gas Production - Produced Water Pond - Netted pit	GAS	Produced water; Oil and gas; Evaporation pond
95699	Oil and Natural Gas Production - Produced Water Pond - Netted pit	GAS	Produced water; Oil and gas; Evaporation pond
95700	Oil and Natural Gas Production - Produced Water Pond - Netted pit	GAS	Produced water; Oil and gas; Evaporation pond
95701	Oil and Natural Gas Production - Produced Water Pond - Netted pit	GAS	Produced water; Oil and gas; Evaporation pond
95702	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95703	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95704	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95705	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95706	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95707	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95708	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95709	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95710	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95711	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95712	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95713	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95714	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95715	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95716	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95717	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95718	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95719	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95720	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95721	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95722	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95723	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95724	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95725	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95726	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95727	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95728	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95729	Oil and Natural Gas Production - Produced Water Pond - actively aerated pond	GAS	Produced water; Oil and gas; Evaporation pond
95730	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95731	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95732	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95733	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95734	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95735	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95736	Oil and Natural Gas Production - Produced Water Pond	GAS	Produced water; Oil and gas; Evaporation pond
95781	Oil and Natural Gas Production - Produced Water Pond – Utah	GAS	Produced water; Oil and gas; Evaporation pond
95782	Oil and Natural Gas Production - Produced Water Pond - Wyoming	GAS	Produced water; Oil and gas; Evaporation pond
95335a	Diesel Exhaust - Heavy-heavy duty truck - 2011 model year corrected	GAS	Diesel Exhaust; Heavy-heavy duty truck; 2011 model year
95784	Gasoline Exhaust - E10 gasoline - Cold Start - 0 oF	GAS	Gasoline Exhaust; E10 gasoline; Cold Start; 0 oF
95785	Gasoline Exhaust - E10 gasoline - Cold Start - 20 oF	GAS	Gasoline Exhaust; E10 gasoline; Cold Start; 20 oF
95786	Gasoline Exhaust - E10 gasoline - Cold Start - 75 oF	GAS	Gasoline Exhaust; E10 gasoline; Cold Start; 75 oF
95787	Gasoline Exhaust - E10 gasoline - FTP75 Composite - 0 oF	GAS	Gasoline Exhaust; E10 gasoline; FTP75 Composite; 0 oF
95788	Gasoline Exhaust - E10 gasoline - FTP75 Composite - 20 oF	GAS	Gasoline Exhaust; E10 gasoline; FTP75 Composite; 20 oF
95789	Gasoline Exhaust - E10 gasoline - FTP75 Composite - 75 oF	GAS	Gasoline Exhaust; E10 gasoline; FTP75 Composite; 75 oF
95790	Gasoline Exhaust - E10 gasoline - US06 Composite - 0 oF	GAS	Gasoline Exhaust; E10 gasoline; US06 Composite; 0 oF

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95791	Gasoline Exhaust - E10 gasoline - US06 Composite - 20 oF	GAS	Gasoline Exhaust; E10 gasoline; US06 Composite; 20 oF
95792	Gasoline Exhaust - E10 gasoline - US06 Composite - 75 oF	GAS	Gasoline Exhaust; E10 gasoline; US06 Composite; 75 oF
CARB3001	CONS PRD- CONSTRUCTION, PANEL, OR FLOOR COVERING ADHESIVE (2010 UPDATE)	GAS	CONS PRD- CONSTRUCTION, PANEL, OR FLOOR COVERING ADHESIVE (2010 UPDATE)
CARB3002	CONS PRD- GENERAL PURPOSE ADHESIVE (2010 UPDATE)	GAS	CONS PRD- GENERAL PURPOSE ADHESIVE (2010 UPDATE)
CARB3003	CONS PRD- AEROSOL ADHESIVE (INCLUDING INDSTRIAL) (2010 UPDATE)	GAS	CONS PRD- AEROSOL ADHESIVE (INCLUDING INDSTRIAL) (2010 UPDATE)
CARB3004	CONS PRD- PIPE CEMENT AND PRIMER (2010 UPDATE)	GAS	CONS PRD- PIPE CEMENT AND PRIMER (2010 UPDATE)
CARB3005	CONS PRD- SEALANT AND CAULKING COMPOUND (2010 UPDATE)	GAS	CONS PRD- SEALANT AND CAULKING COMPOUND (2010 UPDATE)
CARB3006	CONS PRD- BUG AND TAR REMOVER (2010 UPDATE)	GAS	CONS PRD- BUG AND TAR REMOVER (2010 UPDATE)
CARB3007	CONS PRD- AUTO HARD PASTE WAX (2010 UPDATE)	GAS	CONS PRD- AUTO HARD PASTE WAX (2010 UPDATE)
CARB3008	CONS PRD- AUTOMOTIVE INSTANT DETAILER (2010 UPDATE)	GAS	CONS PRD- AUTOMOTIVE INSTANT DETAILER (2010 UPDATE)
CARB3009	CONS PRD- AUTOMOTIVE POLISH,SEALANT,WAX,GLAZE (2010 UPDATE)	GAS	CONS PRD- AUTOMOTIVE POLISH,SEALANT,WAX,GLAZE (2010 UPDATE)
CARB3010	CONS PRD- AUTOMOTIVE RUBBING OR POLISHING COMPOUND (2010 UPDATE)	GAS	CONS PRD- AUTOMOTIVE RUBBING OR POLISHING COMPOUND (2010 UPDATE)
CARB3011	CONS PRD- TIRE CLEANER AND WHEEL CLEANER (2010 UPDATE)	GAS	CONS PRD- TIRE CLEANER AND WHEEL CLEANER (2010 UPDATE)
CARB3012	CONS PRD- AUTOMOTIVE BRAKE CLEANER (2010 UPDATE)	GAS	CONS PRD- AUTOMOTIVE BRAKE CLEANER (2010 UPDATE)
CARB3013	CONS PRD- CARBURETOR OR FUEL-INJECTION AIR INTAKE CLEANER (2010 UPDATE)	GAS	CONS PRD- CARBURETOR OR FUEL-INJECTION AIR INTAKE CLEANER (2010 UPDATE)
CARB3014	CONS PRD- ENGINE DEGREASER (2010 UPDATE)	GAS	CONS PRD- ENGINE DEGREASER (2010 UPDATE)
CARB3015	CONS PRD- TIRE SEALANTS AND INFLATOR (2010 UPDATE)	GAS	CONS PRD- TIRE SEALANTS AND INFLATOR (2010 UPDATE)
CARB3016	CONS PRD- AUTOMOTIVE UNDERCOATINGS - AEROSOL (2010 UPDATE)	GAS	CONS PRD- AUTOMOTIVE UNDERCOATINGS - AEROSOL (2010 UPDATE)
CARB3017	CONS PRD- AUTOMOTIVE WINDSHIELD WASHER FLUID - NON TYPE A AREAS (2010 U)	GAS	CONS PRD- AUTOMOTIVE WINDSHIELD WASHER FLUID - NON TYPE A AREAS (2010 U)
CARB3018	CONS PRD- PAINT REMOVER OR STRIPPER (2010 UPDATE)	GAS	CONS PRD- PAINT REMOVER OR STRIPPER (2010 UPDATE)
CARB3019	CONS PRD- MULTI-PURPOSE SOLVENT AND PAINT THINNER (2010 UPDATE)	GAS	CONS PRD- MULTI-PURPOSE SOLVENT AND PAINT THINNER (2010 UPDATE)
CARB3020	CONS PRD- DISINFECTANTS (ALL FORMS) (2010 UPDATE)	GAS	CONS PRD- DISINFECTANTS (ALL FORMS) (2010 UPDATE)
CARB3021	CONS PRD- SANITIZER (2010 UPDATE)	GAS	CONS PRD- SANITIZER (2010 UPDATE)
CARB3022	CONS PRD- NON-SELECTIVE TERRESTRIAL HERBICIDE (2010 UPDATE)	GAS	CONS PRD- NON-SELECTIVE TERRESTRIAL HERBICIDE (2010 UPDATE)
CARB3023	CONS PRD- FLEA AND TICK INSECTICIDE (2010 UPDATE)	GAS	CONS PRD- FLEA AND TICK INSECTICIDE (2010 UPDATE)
CARB3024	CONS PRD- FLYING BUG INSECTICIDE - AEROSOL (2010 UPDATE)	GAS	CONS PRD- FLYING BUG INSECTICIDE - AEROSOL (2010 UPDATE)
CARB3025	CONS PRD- FLYING BUG INSECTICIDE - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- FLYING BUG INSECTICIDE - NON-AEROSOL (2010 UPDATE)
CARB3026	CONS PRD- WASP OR HORNET INSECTICIDE (2010 UPDATE)	GAS	CONS PRD- WASP OR HORNET INSECTICIDE (2010 UPDATE)
CARB3027	CONS PRD- LAWN AND GARDEN INSECTICIDE (2010 UPDATE)	GAS	CONS PRD- LAWN AND GARDEN INSECTICIDE (2010 UPDATE)

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
CARB3028	CONS PRD- CRAWLING BUG INSECTICIDE - AEROSOL (2010 UPDATE)	GAS	CONS PRD- CRAWLING BUG INSECTICIDE - AEROSOL (2010 UPDATE)
CARB3029	CONS PRD- CRAWLING BUG INSECTICIDE - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- CRAWLING BUG INSECTICIDE - NON-AEROSOL (2010 UPDATE)
CARB3030	CONS PRD- INSECTICIDE FOGGER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- INSECTICIDE FOGGER - AEROSOL (2010 UPDATE)
CARB3031	CONS PRD- INSECT REPELLENT - AEROSOL (2010 UPDATE)	GAS	CONS PRD- INSECT REPELLENT - AEROSOL (2010 UPDATE)
CARB3032	CONS PRD- INSECT REPELLENT - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- INSECT REPELLENT - NON-AEROSOL (2010 UPDATE)
CARB3033	CONS PRD- CARPET AND UPHOLSTERY CLEANER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- CARPET AND UPHOLSTERY CLEANER - AEROSOL (2010 UPDATE)
CARB3034	CONS PRD- CARPET AND UPHOLSTERY CLEANER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- CARPET AND UPHOLSTERY CLEANER - NON-AEROSOL (2010 UPDATE)
CARB3035	CONS PRD- SPOT REMOVER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- SPOT REMOVER - AEROSOL (2010 UPDATE)
CARB3036	CONS PRD- SPOT REMOVER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- SPOT REMOVER - NON-AEROSOL (2010 UPDATE)
CARB3037	CONS PRD- FABRIC PROTECTANT - AEROSOL (2010 UPDATE)	GAS	CONS PRD- FABRIC PROTECTANT - AEROSOL (2010 UPDATE)
CARB3038	CONS PRD- FLOOR WAX STRIPPER (2010 UPDATE)	GAS	CONS PRD- FLOOR WAX STRIPPER (2010 UPDATE)
CARB3039	CONS PRD- GENERAL PURPOSE CLEANER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- GENERAL PURPOSE CLEANER - AEROSOL (2010 UPDATE)
CARB3040	CONS PRD- GENERAL PURPOSE CLEANER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- GENERAL PURPOSE CLEANER - NON-AEROSOL (2010 UPDATE)
CARB3041	CONS PRD- GENERAL PURPOSE DEGREASER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- GENERAL PURPOSE DEGREASER - AEROSOL (2010 UPDATE)
CARB3042	CONS PRD- GENERAL PURPOSE DEGREASER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- GENERAL PURPOSE DEGREASER - NON-AEROSOL (2010 UPDATE)
CARB3043	CONS PRD- GLASS CLEANER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- GLASS CLEANER - AEROSOL (2010 UPDATE)
CARB3044	CONS PRD- GLASS CLEANER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- GLASS CLEANER - NON-AEROSOL (2010 UPDATE)
CARB3045	CONS PRD- METAL POLISH OR CLEANSER (2010 UPDATE)	GAS	CONS PRD- METAL POLISH OR CLEANSER (2010 UPDATE)
CARB3046	CONS PRD- OVEN CLEANER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- OVEN CLEANER - AEROSOL (2010 UPDATE)
CARB3047	CONS PRD- OVEN CLEANER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- OVEN CLEANER - NON-AEROSOL (2010 UPDATE)
CARB3048	CONS PRD- BATHROOM AND TILE CLEANER - AEROSOL (2010 UPDATE)	GAS	CONS PRD- BATHROOM AND TILE CLEANER - AEROSOL (2010 UPDATE)
CARB3049	CONS PRD- BATHROOM AND TILE CLEANER - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- BATHROOM AND TILE CLEANER - NON-AEROSOL (2010 UPDATE)
CARB3050	CONS PRD- LAUNDRY PREWASH (2010 UPDATE)	GAS	CONS PRD- LAUNDRY PREWASH (2010 UPDATE)
CARB3051	CONS PRD- LAUNDRY STARCH OR SIZING (2010 UPDATE)	GAS	CONS PRD- LAUNDRY STARCH OR SIZING (2010 UPDATE)
CARB3052	CONS PRD- DUSTING AID - AEROSOL (2010 UPDATE)	GAS	CONS PRD- DUSTING AID - AEROSOL (2010 UPDATE)
CARB3053	CONS PRD- DUSTING AID - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- DUSTING AID - NON-AEROSOL (2010 UPDATE)
CARB3054	CONS PRD- FLOOR POLISH OR WAX - RESILIENT AND NONRESILIENT (2010 UPDATE)	GAS	CONS PRD- FLOOR POLISH OR WAX - RESILIENT AND NONRESILIENT (2010 UPDATE)
CARB3055	CONS PRD- FLOOR POLISH OR WAX - WOOD (2010 UPDATE)	GAS	CONS PRD- FLOOR POLISH OR WAX - WOOD (2010 UPDATE)

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
CARB3056	CONS PRD- FURNITURE MAINTENANCE PRODUCT - AEROSOL (2010 UPDATE)	GAS	CONS PRD- FURNITURE MAINTENANCE PRODUCT - AEROSOL (2010 UPDATE)
CARB3057	CONS PRD- FURNITURE MAINTENANCE PRODUCT - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- FURNITURE MAINTENANCE PRODUCT - NON-AEROSOL (2010 UPDATE)
CARB3058	CONS PRD- MULTIPURPOSE LUBRICANT (2010 UPDATE)	GAS	CONS PRD- MULTIPURPOSE LUBRICANT (2010 UPDATE)
CARB3059	CONS PRD- SILICONE BASED MULTI-PURPOSE LUBRICANT (2010 UPDATE)	GAS	CONS PRD- SILICONE BASED MULTI-PURPOSE LUBRICANT (2010 UPDATE)
CARB3060	CONS PRD- PENETRANT (2010 UPDATE)	GAS	CONS PRD- PENETRANT (2010 UPDATE)
CARB3061	CONS PRD- SPECIAL PURPOSE LUBRICANT (2010 UPDATE)	GAS	CONS PRD- SPECIAL PURPOSE LUBRICANT (2010 UPDATE)
CARB3062	CONS PRD- SINGLE PHASE AEROSOL AIR FRESHENER (2010 UPDATE)	GAS	CONS PRD- SINGLE PHASE AEROSOL AIR FRESHENER (2010 UPDATE)
CARB3063	CONS PRD- DOUBLE PHASE AEROSOL AIR FRESHENER (2010 UPDATE)	GAS	CONS PRD- DOUBLE PHASE AEROSOL AIR FRESHENER (2010 UPDATE)
CARB3065	CONS PRD- LIQUID OR PUMP AIR FRESHENER (2010 UPDATE)	GAS	CONS PRD- LIQUID OR PUMP AIR FRESHENER (2010 UPDATE)
CARB3066	CONS PRD- CHARCOAL LIGHTER MATERIAL (2010 UPDATE)	GAS	CONS PRD- CHARCOAL LIGHTER MATERIAL (2010 UPDATE)
CARB3067	CONS PRD- AEROSOL COOKING SPRAY (2010 UPDATE)	GAS	CONS PRD- AEROSOL COOKING SPRAY (2010 UPDATE)
CARB3068	CONS PRD- ANTIPERSPIRANT (2010 UPDATE)	GAS	CONS PRD- ANTIPERSPIRANT (2010 UPDATE)
CARB3069	CONS PRD- UNDERARM DEODORANT (2010 UPDATE)	GAS	CONS PRD- UNDERARM DEODORANT (2010 UPDATE)
CARB3070	CONS PRD- ASTRINGENTS AND TONER (2010 UPDATE)	GAS	CONS PRD- ASTRINGENTS AND TONER (2010 UPDATE)
CARB3071	CONS PRD- PERSONAL FRAGRANCE PRODUCT (FRAGRANCE <= 20%) (2010 UPDATE)	GAS	CONS PRD- PERSONAL FRAGRANCE PRODUCT (FRAGRANCE <= 20%) (2010 UPDATE)
CARB3072	CONS PRD- PERSONAL FRAGRANCE PRODUCT (FRAGRANCE > 20%) (2010 UPDATE)	GAS	CONS PRD- PERSONAL FRAGRANCE PRODUCT (FRAGRANCE > 20%) (2010 UPDATE)
CARB3073	CONS PRD- HAIR SPRAY (2010 UPDATE)	GAS	CONS PRD- HAIR SPRAY (2010 UPDATE)
CARB3074	CONS PRD- HAIR SHINE (2010 UPDATE)	GAS	CONS PRD- HAIR SHINE (2010 UPDATE)
CARB3075	CONS PRD- NAIL COATING (2010 UPDATE)	GAS	CONS PRD- NAIL COATING (2010 UPDATE)
CARB3076	CONS PRD- RUBBING ALCOHOL (2010 UPDATE)	GAS	CONS PRD- RUBBING ALCOHOL (2010 UPDATE)
CARB3077	CONS PRD- HEAVY-DUTY HAND CLEANSER OR SOAP (2010 UPDATE)	GAS	CONS PRD- HEAVY-DUTY HAND CLEANSER OR SOAP (2010 UPDATE)
CARB3078	CONS PRD- DEODORANT BODY SPRAY (2010 UPDATE)	GAS	CONS PRD- DEODORANT BODY SPRAY (2010 UPDATE)
CARB3079	CONS PRD- DRYER SHEET (2010 UPDATE)	GAS	CONS PRD- DRYER SHEET (2010 UPDATE)
CARB3080	CONS PRD- ODOR REMOVER OR ELIMINATOR (2010 UPDATE)	GAS	CONS PRD- ODOR REMOVER OR ELIMINATOR (2010 UPDATE)
CARB3081	CONS PRD- WINDSHIELD WATER REPELLENT (2010 UPDATE)	GAS	CONS PRD- WINDSHIELD WATER REPELLENT (2010 UPDATE)
CARB3082	CONS PRD- FLOOR MAINTENANCE PRODUCT (2010 UPDATE)	GAS	CONS PRD- FLOOR MAINTENANCE PRODUCT (2010 UPDATE)
CARB3083	CONS PRD- TEMPORARY HAIR COLOR - AEROSOL (2010 UPDATE)	GAS	CONS PRD- TEMPORARY HAIR COLOR - AEROSOL (2010 UPDATE)
CARB3084	CONS PRD- INSULATING AND SEALING FOAM (2010 UPDATE)	GAS	CONS PRD- INSULATING AND SEALING FOAM (2010 UPDATE)
CARB3085	CONS PRD- HAND SANITIZER (2010 UPDATE)	GAS	CONS PRD- HAND SANITIZER (2010 UPDATE)
CARB3086	CONS PRD- PERSONAL CARE WIPES (2010 UPDATE)	GAS	CONS PRD- PERSONAL CARE WIPES (2010 UPDATE)

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
CARB3087	CONS PRD- FABRIC PROTECTANT - NON-AEROSOL (2010 UPDATE)	GAS	CONS PRD- FABRIC PROTECTANT - NON-AEROSOL (2010 UPDATE)
CARB3088	CONS PRD- SUN SCREEN AND TANNING PRODUCT (2010 UPDATE)	GAS	CONS PRD- SUN SCREEN AND TANNING PRODUCT (2010 UPDATE)
CARB3089	CONS PRD- FABRIC SOFTENER (2010 UPDATE)	GAS	CONS PRD- FABRIC SOFTENER (2010 UPDATE)
CARB3090	CONS PRD- MOTHBALLS (2010 UPDATE)	GAS	CONS PRD- MOTHBALLS (2010 UPDATE)
CARB3091	CONS PRD- BRUSH CLEANER (2010 UPDATE)	GAS	CONS PRD- BRUSH CLEANER (2010 UPDATE)
CARB3092	CONS PRD- AUTOMOTIVE WINDSHIELD WASHER FLUID - TYPE A AREAS (2010 UPDT)	GAS	CONS PRD- AUTOMOTIVE WINDSHIELD WASHER FLUID - TYPE A AREAS (2010 UPDT)
CARB3093	CONS PRD- PRESSURIZED GAS DUSTER (2010 UPDATE)	GAS	CONS PRD- PRESSURIZED GAS DUSTER (2010 UPDATE)
CARB3094	CONS PRD- WITCH HAZEL (2010 UPDATE)	GAS	CONS PRD- WITCH HAZEL (2010 UPDATE)
CARB3095	CONS PRD- MOTOR VEHICLE WASH AND CLEANER (2010 UPDATE)	GAS	CONS PRD- MOTOR VEHICLE WASH AND CLEANER (2010 UPDATE)
CARB3096	CONS PRD- ALL OTHER ADHESIVES (2010 UPDATE)	GAS	CONS PRD- ALL OTHER ADHESIVES (2010 UPDATE)
CARB3097	CONS PRD- OTHER SEALANTS (2010 UPDATE)	GAS	CONS PRD- OTHER SEALANTS (2010 UPDATE)
CARB3098	CONS PRD- OTHER CLEANERS AND DEGREASERS (2010 UPDATE)	GAS	CONS PRD- OTHER CLEANERS AND DEGREASERS (2010 UPDATE)
CARB3100	CONS PRD- OTHER LAUNDRY (2010 UPDATE)	GAS	CONS PRD- OTHER LAUNDRY (2010 UPDATE)
CARB3101	CONS PRD- OTHER MISC HOUSEHOLD PRODUCTS (2010 UPDATE)	GAS	CONS PRD- OTHER MISC HOUSEHOLD PRODUCTS (2010 UPDATE)
CARB3102	CONS PRD- OTHER PERSONAL CARE PRODUCTS (2010 UPDATE)	GAS	CONS PRD- OTHER PERSONAL CARE PRODUCTS (2010 UPDATE)
CARB3103	CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)	GAS	CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
CARB3104	CONS PRD- OTHER VEHICLE MAINTENANCE PRODUCTS (2010 UPDATE)	GAS	CONS PRD- OTHER VEHICLE MAINTENANCE PRODUCTS (2010 UPDATE)
CARB3105	CONS PRD- MISC ART AND OFFICE PRODUCTS (2010 UPDATE)	GAS	CONS PRD- MISC ART AND OFFICE PRODUCTS (2010 UPDATE)
CARB3106	CONS PRD- OTHER LAWN AND GARDEN PRODUCTS (2010 UPDATE)	GAS	CONS PRD- OTHER LAWN AND GARDEN PRODUCTS (2010 UPDATE)
CARB3107	CONS PRD- OTHER AIR FRESHENERS (2010 UPDATE)	GAS	CONS PRD- OTHER AIR FRESHENERS (2010 UPDATE)
CARB3901	2004 Architectural Coatings - solvent based - 2005 survey	GAS	2004 Architectural Coatings - solvent based - 2005 survey
CARB3902	2004 Architectural Coatings - water based - 2005 survey	GAS	2004 Architectural Coatings - water based - 2005 survey
G4420	Rice Straw Burning Gap-filled from 4420	GAS	Rice Straw Burning; Agricultural Burning; Prescribed Burning
G4421	Wheat Straw Burning Gap-filled from 4421	GAS	Wheat Straw Burning; Agricultural Burning; Prescribed Burning
G8746	Rice Straw and Wheat Straw Burning Composite of G4420 and G4421	GAS	Rice and Wheat Straw Burning; Agricultural Burning; Prescribed Burning
G95223TOG	Poultry Production - Average of Production Cycle with gapfilled methane and ethane	GAS	Poultry Production
G95240TOG	Beef Cattle Farm and Animal Waste with gapfilled methane and ethane	GAS	Beef Cattle Farm; Animal Waste
G95241TOG	Swine Farm and Animal Waste with gapfilled methane and ethane	GAS	Swine Farm; Animal Waste
G95467	Residential Wood Combustion - Fireplace, Softwood	GAS	Residential Wood Combustion; Fireplace; Softwood
G95468	Residential Wood Combustion - Fireplace, Hardwood	GAS	Residential Wood Combustion; Fireplace; Hardwood
G95469	Residential Wood Combustion – Noncatalytic Woodstove, Hardwood	GAS	Residential Wood Combustion; Noncatalytic Woodstove; Hardwood
G95470	Residential Wood Combustion - Fireplace, Synthetic	GAS	Residential Wood Combustion; Fireplace; Synthetic
SUG01	Sugar Cane Pre-Harvest Burning Florida	GAS	Sugar cane; Biomass burning

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
SUG02	Sugar Cane Pre-Harvest Burning Mexico	GAS	Sugar cane; Biomass burning
SUG03	Sugar Cane Pre-Harvest Burning Florida and Mexico Composite	GAS	Sugar cane; Biomass burning
100VBS	Onroad gasoline vehicle cold-start with VBS	GAS-VBS	On-road gasoline exhaust-Cold UC, VBS
101VBS	Onroad gasoline vehicle hot-start with VBS	GAS-VBS	On-road gasoline exhaust-Hot start, VBS
102VBS	Gas-turbine (aircraft) engine supplemented with aircraft profile 5565 with VBS	GAS-VBS	Aircraft engine exhaust-4% thrust, VBS
103VBS	Heavy Duty diesel with DPF, combination of previous measurements with VBS	GAS-VBS	On-road non-DPF diesel vehicle exhaust, VBS

Table A-2. List of New PM Profiles (Type = PM, PM-AE6, PM-VBS) Added to the SPECIATE 5.0 Database

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95759	Residential Wood Combustion - non-EPA Certified Woodstove, Pine	PM	Residential Wood Combustion; Woodstove, Pine
95760	Residential Wood Combustion - non-EPA Certified Woodstove, Almond	PM	Residential Wood Combustion; Woodstove, Almond
95761	Residential Wood Combustion - non-EPA Certified Woodstove, Almond	PM	Residential Wood Combustion; Woodstove, Almond
95762	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine	PM	Residential Wood Combustion; Woodstove, Pine
95763	Residential Wood Combustion - Fireplace, Oak	PM	Residential Wood Combustion; Fireplace, Oak
95764	Residential Wood Combustion - Fireplace, Oak	PM	Residential Wood Combustion; Fireplace, Oak
95765	Residential Wood Combustion - Fireplace, Juniper	PM	Residential Wood Combustion; Fireplace, Juniper
95766	Residential Wood Combustion - Fireplace, Juniper	PM	Residential Wood Combustion; Fireplace, Juniper
95767	Residential Wood Combustion - Fireplace, Juniper	PM	Residential Wood Combustion; Fireplace, Juniper
95768	Residential Wood Combustion - Fireplace, Oak Composite	PM	Residential Wood Combustion; Fireplace, Oak Composite
95769	Residential Wood Combustion - Fireplace, Juniper Composite	PM	Residential Wood Combustion; Fireplace, Juniper Composite
95770	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine Composite	PM	Residential Wood Combustion; Woodstove, Pine Composite
95771	Residential Wood Combustion - Non-EPA Certified Woodstove, Almond Composite	PM	Residential Wood Combustion; Woodstove, Almond Composite
95772	Residential Wood Combustion - Fireplace-Juniper, Woodstove-Pine, Lake Tahoe Study Composite	PM	Residential Wood Combustion; Woodstove, Softwood Composite
95773	Residential Wood Combustion - Composite of fireplace burning oak and Woodstoves burning almond	PM	Residential Wood Combustion; Composite of fireplace burning oak and Woodstoves burning almond
95774	Residential Wood Combustion - Fireplace, Oak and Juniper Composite	PM	Residential Wood Combustion; Fireplace, Oak and Juniper Composite
95775	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine and Almond Composite	PM	Residential Wood Combustion; Woodstove, Pine and Almond Composite
95776	Residential Wood Combustion - Composite of fireplace and woodstove burning oak, juniper, pine, or almond	PM	Residential Wood Combustion; Composite of fireplace and woodstove burning oak, juniper, pine, almond
95777	Paved Road Dust	PM	Paved Road Dust
95778	Paved Road Dust	PM	Paved Road Dust
95779	Paved Road Dust	PM	Paved Road Dust
95780	Paved Road Dust	PM	Paved Road Dust
95463	Residential Wood Combustion - Fireplace, Softwood	PM-AE6	Residential Wood Combustion; Fireplace; Softwood
95464	Residential Wood Combustion - Fireplace, Hardwood	PM-AE6	Residential Wood Combustion; Fireplace; Hardwood
95465	Residential Wood Combustion – Noncatalytic Woodstove, Hardwood	PM-AE6	Residential Wood Combustion; Noncatalytic Woodstove; Hardwood
95466	Residential Wood Combustion - Fireplace, Synthetic	PM-AE6	Residential Wood Combustion; Fireplace; Synthetic
95475	Composite -Refinery Fuel Gas and Natural Gas Combustion	PM-AE6	AE6; Composite - Natural Gas Combustion
95501	Agricultural Burning - Wheat Straw – China	PM-AE6	Agricultural Burning; Wheat Straw
95502	Agricultural Burning - Rice Straw – China	PM-AE6	Agricultural Burning; Rice Straw
95503	Agricultural Burning - Corn Stalk – China	PM-AE6	Agricultural Burning; Corn Stalk

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95504	Agricultural Burning Composite - Wheat Straw, Rice Straw and Corn Stalk - China	PM-AE6	Agricultural Burning; Composite
95514	Coal Combustion - Prater Creek Coal	PM-AE6	Coal Combustion; Prater Creek Coal; Pulverized Coal
95515	Coal Combustion - Prater Creek w/biomass	PM-AE6	Coal Combustion; Prater Creek with biomass; Pulverized Coal
95516	Coal Combustion - Black Thunder Coal	PM-AE6	Coal Combustion; Black Thunder Coal; Pulverized Coal
95517	Coal Combustion - Bailey Mine Coal	PM-AE6	Coal Combustion; Bailey Mine Coal; Pulverized Coal
95518	Coal Combustion - Western Canadian lignite	PM-AE6	Coal Combustion; Western Canadian lignite
95519	Unpaved Road Dust – Detroit	PM-AE6	Unpaved Road Dust; Detroit
95520	Urban Soil – Detroit	PM-AE6	Urban Soil; Detroit
95521	Agricultural Soil – Detroit	PM-AE6	Agricultural Soil; Detroit
95522	Paved Road Dust – Cleveland	PM-AE6	Paved Road Dust; Cleveland
95523	Unpaved Road Dust – Cleveland	PM-AE6	Unpaved Road Dust; Cleveland
95524	Urban Soil – Cleveland	PM-AE6	Urban Soil; Cleveland
95525	Agricultural Soil – Cleveland	PM-AE6	Agricultural Soil; Cleveland
95526	Paved Road Dust - Saint Louis	PM-AE6	Paved Road Dust; Saint Louis
95527	Unpaved Road Dust - Saint Louis	PM-AE6	Unpaved Road Dust; Saint Louis
95528	Urban Soil - Saint Louis	PM-AE6	Urban Soil; Saint Louis
95529	Paved Road Dust – Chicago	PM-AE6	Paved Road Dust; Chicago
95530	Unpaved Road Dust – Chicago	PM-AE6	Unpaved Road Dust; Chicago
95531	Construction Soil – Chicago	PM-AE6	Construction Soil; Chicago
95532	Agricultural Soil – Cincinnati	PM-AE6	Agricultural Soil; Cincinnati
95533	Paved Road Dust - San Joaquin Valley	PM-AE6	Paved Road Dust; San Joaquin Valley
95534	Paved Road Dust - Los Angeles	PM-AE6	Paved Road Dust; Los Angeles
95535	Paved Road Dust – California	PM-AE6	Paved Road Dust; California
95737	Residential Wood Combustion - non-EPA Certified Woodstove, Pine	PM-AE6	Residential Wood Combustion; Woodstove, Pine
95738	Residential Wood Combustion - non-EPA Certified Woodstove, Almond	PM-AE6	Residential Wood Combustion; Woodstove, Almond
95739	Residential Wood Combustion - non-EPA Certified Woodstove, Almond	PM-AE6	Residential Wood Combustion; Woodstove, Almond
95740	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine	PM-AE6	Residential Wood Combustion; Woodstove, Pine
95741	Residential Wood Combustion - Fireplace, Oak	PM-AE6	Residential Wood Combustion; Fireplace, Oak
95742	Residential Wood Combustion - Fireplace, Oak	PM-AE6	Residential Wood Combustion; Fireplace, Oak
95743	Residential Wood Combustion - Fireplace, Juniper	PM-AE6	Residential Wood Combustion; Fireplace, Juniper
95744	Residential Wood Combustion - Fireplace, Juniper	PM-AE6	Residential Wood Combustion; Fireplace, Juniper
95745	Residential Wood Combustion - Fireplace, Juniper	PM-AE6	Residential Wood Combustion; Fireplace, Juniper
95746	Residential Wood Combustion - Fireplace, Oak Composite	PM-AE6	Residential Wood Combustion; Fireplace, Oak Composite
95747	Residential Wood Combustion - Fireplace, Juniper Composite	PM-AE6	Residential Wood Combustion; Fireplace, Juniper Composite

PROFILE CODE	PROFILE_NAME	PROFILE TYPE	KEYWORD
95748	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine Composite	PM-AE6	Residential Wood Combustion; Woodstove, Pine Composite
95749	Residential Wood Combustion - Non-EPA Certified Woodstove, Almond Composite	PM-AE6	Residential Wood Combustion; Woodstove, Almond Composite
95750	Residential Wood Combustion - Fireplace-Juniper, Woodstove-Pine, Lake Tahoe Study Composite	PM-AE6	Residential Wood Combustion; Woodstove, Softwood Composite
95751	Residential Wood Combustion - Composite of fireplace burning oak and Woodstoves burning almond	PM-AE6	Residential Wood Combustion; Composite of fireplace burning oak and Woodstoves burning almond
95752	Residential Wood Combustion - Fireplace, Oak and Juniper Composite	PM-AE6	Residential Wood Combustion; Fireplace, Oak and Juniper Composite
95753	Residential Wood Combustion - Non-EPA Certified Woodstove, Pine and Almond Composite	PM-AE6	Residential Wood Combustion; Woodstove, Pine and Almond Composite
95754	Residential Wood Combustion - Composite of fireplace and woodstove burning oak, juniper, pine, or almond	PM-AE6	Residential Wood Combustion; Composite of fireplace and woodstove burning oak, juniper, pine, almond
95756	Paved Road Dust	PM-AE6	Paved Road Dust
95757	Paved Road Dust	PM-AE6	Paved Road Dust
95758	Paved Road Dust	PM-AE6	Paved Road Dust
95783	Aircraft Exhaust - Composite - AE6	PM-AE6	Aircraft Exhaust; Jet Engine Exhaust
3766AE6	Forest Fire - AE6	PM-AE6	Vegetative Burning; Forest Fire
5675AE6	Marine Vessel - Auxiliary Engine - Marine Gas Oil - with AE6 species added	PM-AE6	Marine Vessel; Auxiliary Engine; Marine Gas Oil
95125a	Gas-fired boiler exhaust	PM-AE6	AE6; Gas-fired boiler exhaust
95126a	Gas-fired process heater exhaust	PM-AE6	AE6; Gas-fired process heater exhaust
95127a	Gas-fired internal combustion combined cycle/cogeneration plant exhaust	PM-AE6	AE6; Gas-fired internal combustion combined cycle/cogeneration plant exhaust
95128a	Institutional boiler exhaust fueled with No. 6 fuel oil	PM-AE6	AE6; Institutional boiler exhaust fueled with No. 6 oil
8873VBS	Aircraft Exhaust, VBS	PM-VBS	Aircraft Exhaust, VBS
8992VBS	Light Duty Gasoline Vehicles-Start, VBS	PM-VBS	Gasoline Vehicles Exhaust; Start; Volatility Basis Set (VBS)
8993VBS	Light-duty Gasoline Vehicles Exhaust - Stabilized Running, VBS	PM-VBS	Gasoline Vehicles Exhaust; Hot Stabilized Running
8994VBS	Conventional Diesel Exhaust - Idle Cycle, VBS	PM-VBS	Conventional Diesel Exhaust; Idle
8995VBS	Conventional Diesel Exhaust - Transient Cycle, VBS	PM-VBS	Conventional Diesel Exhaust; Hot Stabilized Running
8996VBS	Diesel Exhaust - Heavy-heavy duty truck - 2007 model year with NCOM, VBS	PM-VBS	2007 to 2009 Heavy-Duty Diesel Exhaust

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 THC method using 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.

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

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

Chemical Name	Weight Percent	CAS
1,1-DIMETHYLCYCLOHEXANE	0.26	590669
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

Chemical Name	Weight Percent	CAS
4-METHYLUNDECANE	0.12	2980690
(1-METHYLPROPYL)BENZENE	0.11	135988
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

Chemical Name	Weight Percent	CAS
2,2-DIMETHYLHEPTANE	0.03	1071267
METHYL ISOBUTYL KETONE	0.03	108101
2,7-DIMETHYLDECANE	0.03	99067
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

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

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.

* 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 semi-volatile 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 semi-volatile 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
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

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
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
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

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
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
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

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
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
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

Species ID	Molecular Weight	Chemical Name	CAS	Gas Phase (µg/km)	Particle Phase (µg/km)	Mass Fraction in Gas	Mass Fraction in PM
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
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

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

APPENDIX E. Profile Quality Criteria Evaluation

The Quality Score (QSCORE) provide an evaluation framework to easily recognize and assign value points to indicators of a strong, well planned and executed study, which is presented in a complete and logical manner. The presentation of air emission profile data can be in the form of a peer-reviewed publication, or report.

The evaluation framework is meant to guide the reviewer to assign quality value points to the areas of the study deemed most important for use in SPECIATE. The framework is meant to be comprehensive, but should also be easy to understand and apply, not rigid and overly detailed. A point to each question adds-up to an evaluation score. An ideal point score would have 30 (Data from Measurements) or 29 (Data from other Methods) desired criteria (points). Each point or points is additive, influencing, but not necessarily distinguishing the study. The publication or report should be ranked as high as possible for inclusion into the SPECIATE database. The QSCORE total points are valued as follows:

20-30 = excellent
12-19 = good
5-11 = fair
<4 = poor

Each numerical ranking (QSCORE) is added to the SPECIATE Database.

DATA FROM MEASUREMENTS - (Ideal score of 30)

No.	Question	Total Points
1	Are data from a peer-reviewed publication?	1
2	Is the source U.S. based or does it relate to a National Emissions Inventory (NEI) source?	1
3	Is the author well known or affiliated with a well-known research organization in conducting speciated source measurements?	1
4	Is the emission source current, are up-to-date technologies employed (collection, measurement, analysis)?	1
5	Is subject source identified as "priority" source (see, for example, the study: Bray, et. al.[1])	1
6	Were data collected under an established quality system or sufficiently addressed /are QA/QC activities associated with the data collection/measurements included in the publication or supplementary information?	1
7	Sampling Design	
7a	Is the sampling design discussed logically (logic behind the experiments)?	1
7b	Are the data limitations clear (i.e., can the reviewer easily figure them out or are they explicitly stated)?	1
7c	Are assumptions clearly stated? (e.g., fireplace is representative of typical fireplace found throughout the country	1
7d	Are samples capturing the natural variability of the sources?	1
8	Measurement Methodologies	
8a	Is measurement instrumentation presented or referenced?	1
8b	Are the data limitations clear?	1

8c	Were measurements taken using standard methods [EPA, National Institute of Standards and Technology (NIST)], and applicable/up-to-date technologies, methods, and instrumentation?	1
8d	Are replicate measurements done (duplicate or triplicate)? (Measurement methods using duplicate or triplicate collection implies that the study payed attention to data accuracy, representation and reproducibility. This attention should be viewed as an advantage.)	1
9	Data reduction procedures (statistics)	
9a	Are standard deviations (SDs) presented in the paper? (SDs are needed in the profile or we would contact the PI to get it.)	1
9b	Are SDs acceptable for the type of source and pollutants measured?	1
9c	Are the data ready for listing? (i.e., data are already in emission factor form, not in need of conversion or clarification; units consistently used throughout the publication; appropriate number of significant figures reported?)	1
9d	Is there complete speciation data of PM or organic gas provided? For organic gas, does the profile include a total amount of gaseous organic compounds (TOG), TOG should include (1) methane; (2) alkanes, alkenes and aromatic VOC; (3) alcohols; (4) aldehydes. $PM_{2.5}$ should include critical pollutants such as (1) EC and OC; (2) sulfate/nitrate/$NH4^+$ ions; (3) metals/inorganics. Higher scores are given if PAHs and SVOCs are also available.	1-10
10	The overall evaluation should ask; is the paper transparent with regards to describing sampling, test methods and data manipulation? Did the clarity and purpose of this paper leave a positive impression? (This element is meant to be based on the EPA reviewer's impression of the paper, not a hard-fast scale, and may vary from one reviewer to another.)	1-3

1. Bray, et. al. 2019. Bray, C.D., Strum, M., Simon, H., Riddick, L., Kosusko, M., Menetrez, M., Hays, M.D., Rao, V., 2019. An Assessment of Important SPECIATE Profiles in the EPA Emissions Modeling Platform and Current Data Gaps. Atmospheric Environment 207, 93-104. DOI: 10.1016/j.atmosenv.2019.03.013

DATA FROM OTHER METHODS (Blended) (Ideal score of 29)

OTHER METHODS: Any paper where the researches did not directly measure what they report in the paper. Examples of other methods: Urbanski 2014 (putting together others' work), profile for flares (FLR99) that estimated the composition from a test of propylene.

No.	Question	Total Points
1	Are data from a peer-reviewed publication?	1
2	Is the source U.S. based or does it relate to a National Emissions Inventory (NEI) source?	1
3	Is the author well known or affiliated with a well-known research organization in conducting speciated source measurements or analyses?	1

4	Is the emission source current, are up-to-date technologies employed (collection, measurement, analysis)?	1
5	Is subject source identified as "priority" source (see, for example, the study: Bray, et. al.[1])	1
6	Composite Data Development	
6a	Are data based on an established, acceptable methodology?	2
6b	If any of the values or data are based on assumptions or calculations are they clearly documented?	2
6c	Was post-processing used for the data? If so, is it novel, reasonable or widely accepted?	2
7	Is there complete speciation data of PM or organic gas provided? For organic gas, does the profile include a total amount of gaseous organic compounds (TOG), TOG should include (1) methane; (2) alkanes, alkenes and aromatic VOC; (3) alcohols; (4) aldehydes. $PM_{2.5}$ should include critical pollutants such as (1) EC and OC; (2) sulfate/nitrate/$NH4^+$ ions; (3) metals/inorganics. Higher scores are given if PAHs and SVOCs are also available.	1-10
8	Are assumptions clearly stated? (i.e., fireplace is representative of typical fireplace found throughout the country)	2
9	Data reduction procedures (statistics)	
9a	Are standard deviations (SDs) presented in the paper? (SDs are needed in the profile or we would contact the PI to get it.)	1
9b	Are SDs acceptable for the type of source and pollutants measured?	1
9c	Are the data ready for listing? (i.e., data are already in emission factor form, not in need of conversion or clarification; units consistently used throughout the publication; appropriate number of significant figures reported?)	1
10	The overall evaluation should ask; is the paper transparent with regards to describing sampling, test methods and data manipulation? Did the clarity and purpose of this paper leave a positive impression? (This element is meant to be based on the EPA reviewer's impression of the paper, not a hard-fast scale, and may vary from one reviewer to another.)	1-3

1. Bray, et. al. 2019. Bray, C.D., Strum, M., Simon, H., Riddick, L., Kosusko, M., Menetrez, M., Hays, M.D., Rao, V., 2019. An Assessment of Important SPECIATE Profiles in the EPA Emissions Modeling Platform and Current Data Gaps. Atmospheric Environment 207, 93-104. DOI: 10.1016/j.atmosenv.2019.03.013

APPENDIX F. Description of Three Profile Categorization Fields

The SPECIATE Workgroup added three profile categorization fields to the PROFILES table to provide readily searchable metadata about the emission source covered by the profile. The fields describe the emission source in terms of emission generation mechanism (level 1), sector and/or equipment (level 2) and fuel and/or product (level 3). These categorization fields are added to help users to identify and group profiles from similar sources and search for profiles. The categorization has been developed for use in the downstream processing of PM speciation profiles for air quality modeling. Currently, profiles for the AE6 mechanism for CMAQ must be created manually and then put into SPECIATE. Efforts have begun to enhance the Speciation Tool, a software program which creates model-ready profiles for input into emissions modeling software, to create AE6 mechanism profiles. This tool will use the profile category fields to assign the appropriate organic matter to organic carbon ratio (OM-to-OC ratio) which is necessary for computing the species needed for AE6 PM profiles. This ratio is dependent on the type of source and will be able to be assigned using the 3 categorization fields.

Three profile categorization fields are used and described as follows:

1) CATEGORY_LEVEL_1_Generation_Mechanism: This is the mechanism by which emissions are generated by the emissions source. There are nine options for this field: Ash, Atomization, Background-air, Chemical Reaction, Combustion, Dust, Microbial, Miscellaneous, and Volatilization.

    a. Ash (PM only): The particulate byproduct created from combustion or chemical reaction. Examples are (1) the sample of baghouse dust crated from steel plant desulfurization unit or (2) coal fly ash

    b. Atomization (PM only): The breaking up of liquid into droplets. It is used for spraying liquid coatings.

    c. Background-air: A measurement of ambient air

    d. Chemical Reaction: The emissions are the result of a chemical reaction. While this may also overlap with combustion, we use this for processes that are not solely combustion such as catalytic cracking, galvanizing, some specific chemical processes, and reactor effluent

    e. Combustion: Burning a fuel or product. It is also used it for all types of cooking (charbroiling, frying, stir frying, cooking on a wood fire and smoking). We use for emissions coming from devices typically used for combustion such as boilers, process heaters, engines, kilns, sinter processes, smelting processes, foundries, furnaces, mobile source exhaust and all types of biomass burning. This is the most commonly used level 1 category.

    f. Dust (PM only): The result of forming particles from mechanical processes such as tilling or otherwise disturbing soil. It also includes dust formed on roads which could include the entrainment of dust on the road as well as the dust deposited from the tailpipe. Other examples include the storage or movement of granulated material such as grain elevators, coal piles etc.

    g. Microbial: Biological decomposition of material. This includes emissions from animal waste and non-combustion waste treatment, fermentation and silage.

    h. Miscellaneous: Variety of different categories. Used for the overall average composite profiles.

    i. Volatilization: Emissions that are caused by volatilizing (and for PM re-condensing) a material. This includes emissions from storage tanks, solvents, fugitive leaks and even metal

processes that involve volatilization due to heating such as welding. For sector-specific composite profiles that combine many emission generation mechanisms, e.g., "Pulp and paper," volatilization was chosen as it is likely the most common emission generation mechanism across the whole facility.

2) CATEGORY_LEVEL_2_Sector_Equipment: This category provides more detail on the emissions generation category by including the sector and/or equipment or process used to generate the emissions. Including the equipment is important for the AE6, since a wood fired boiler is assumed to have a different (OM-to-OC ratio) from biomass burning or prescribed fire, if known the type of industry or non-industrial sector such as chemical manufacturing, mineral products, metals, waste treatment, and agriculture. In addition, the equipment, if known, is also included. Where there are multiple descriptors such as sector, equipment or multiple pieces or equipment, they are separated by semicolons. There are about 200 unique combinations of sector and/or equipment. Examples include: "biomass burning; prescribed fire", "chemical manufacturing; rail car or truck cleaning" and "electric generation; boiler." Often a sector is not known, so level 2 may be just a piece of equipment or process such as "boiler." For mobile sources, level 2 includes "mobile" as the first term and then "onroad" or "nonroad" or other mobile type ("aircraft", "marine") as the second term. The higher-level detail within those categories, e.g. "onroad; light-duty," is provided for some situations but not all, due to the amount of detail that can be readily provided. Also, some profiles may be based on tunnel studies where there may be a mix of vehicle types or there may be composite profiles that could also mix types. Miscellaneous is used if there are a large number of sectors/equipment involved (e.g., oil combustion) or if the profile is an overall default that is not source specific.

3) CATEGORY_LEVEL_3_ Fuel_Product: This category provides the highest level of detail for the profile categorization. For combustion profiles the fuel is provided. That fuel could be a detailed tree species (or list of them, separated by semicolons) or a generic fuel such as "oil" where additional specificity of fuel type is not provided by the available metadata. In many cases the level 3 value is a particular chemical (product of a chemical manufacturing process) or metal product being produced by the emissions process described by the profile. There are nearly 500 unique values. Miscellaneous is used if there are a large number of products or they are not known.

It should be noted that for SPECIATE 5.0 we have populated these category fields for all GAS and the subset of PM, PM-Simplified, PM-VBS and PM-AE6 that are in the 0 to 2.5 micrometers size range.

APPENDIX G. Protocol for Developing AE6-ready $PM_{2.5}$ Speciation Profiles for Inclusion in SPECIATE

Background and Purpose

SPECIATE is the EPA's repository of volatile organic gas and particulate matter (PM) speciation profiles of air pollution sources. Among the many uses of speciation data, these emission source profiles are used to create speciated emissions inventories for photochemical air quality modeling. In particular, volatile organic compounds (VOC) and $PM_{2.5}$ from emission inventories are speciated into the model species required by the chemical and aerosol mechanisms. This document concerns $PM_{2.5}$ profiles used for air quality modeling.

SPECIATE houses different types of $PM_{2.5}$ profiles: PM, PM-SIMPLIFIED, PM-AE6 and PM-VBS. Profiles of type PM contain all the species provided by a measurement study or a combination (composite) of measurement studies. The other PM profile types are profiles derived from a measurement study or composite in order to provide the species required for an air quality modeling aerosol mechanism. The PM-SIMPLIFIED profiles are for the AE5 aerosol mechanism and are computed by keeping only AE5 species (elemental carbon, organic carbon, sulfate and nitrate) and creating a PM Other species calculated as the 100 – sum of AE5 species' weight percent. The PM-AE6 and PM-VBS aerosol mechanisms have additional species not typically measured and that need to be computed. The PM-AE6 profiles include non-carbon organic mass (PNCOM) and/or water (PH2O). The PM-AE6 profiles were first put into the SPECIATE database in SPECIATE 4.3 (series 91XXX) by Reff, et.al. (2009)[1]. They were developed by compositing pre-existing SPECIATE profiles, computing PNCOM and PH2O and ensuring mass conservation. Documentation on the steps taken are provided in the supplemental information of Reff, et. al. (2009). Since that initial work, there have been additional $PM_{2.5}$ speciation data published in the literature for which SPECIATE developers used Reff's approach so that they could be used in the AE6 aerosol mechanism.

The Speciation Tool is software that creates a complete set of emissions modeling ready profiles for input into SMOKE from the profiles in SPECIATE. For AE6 profiles, the Speciation Tool takes the subset of SPECIATE profiles in which the additional species for AE6 were computed (i.e., "AE6-ready" profiles), maps the species IDs in the SPECIATE profile to the AE6 species names and creates "PM Other" (the remainder of the mass not assigned to AE6 species) as 100 – sum of AE6 species. The ability for the Speciation Tool to create AE6 profiles for the modeling allows SPECIATE developers to include AE6-ready profiles that contain all of the measured species plus the additional calculated species so that only one version of the profile needs to go into the SPECIATE database. EPA is also developing the capability for the Speciation Tool to create AE6 profiles from a profile type of PM. This will allow SPECIATE developers to rely on the Speciation Tool to perform the calculations rather than having to do them manually and put the resulting AE6 profile into the SPECIATE database.

The purpose of this protocol is to document the procedure for creating AE6-ready profiles by either of 2 ways (1) performing additional calculations on the measured or composited data and including the AE6-ready profile in SPECIATE, or 2) through running the Speciation tool on PM profiles in SPECIATE. In either way, the creation of these would largely follow the approach in Reff et. al. This will ensure more consistency and transparency in AE6 profiles that are put into SPECIATE or computed by the Speciation Tool. Changes to the Reff et al. approach will be identified.

[1] "Emissions Inventory of $PM_{2.5}$ Trace Elements across the United States"; Adam Reff, Prakash V. Bhave, Heather Simon, Thompson G. Pace, George A. Pouliot, J. David Mobley, and Marc Houyoux; *Environmental Science & Technology* **2009** *43* (15), 5790-5796; DOI: 10.1021/es802930x (Supplemental Information)

AE6 Species

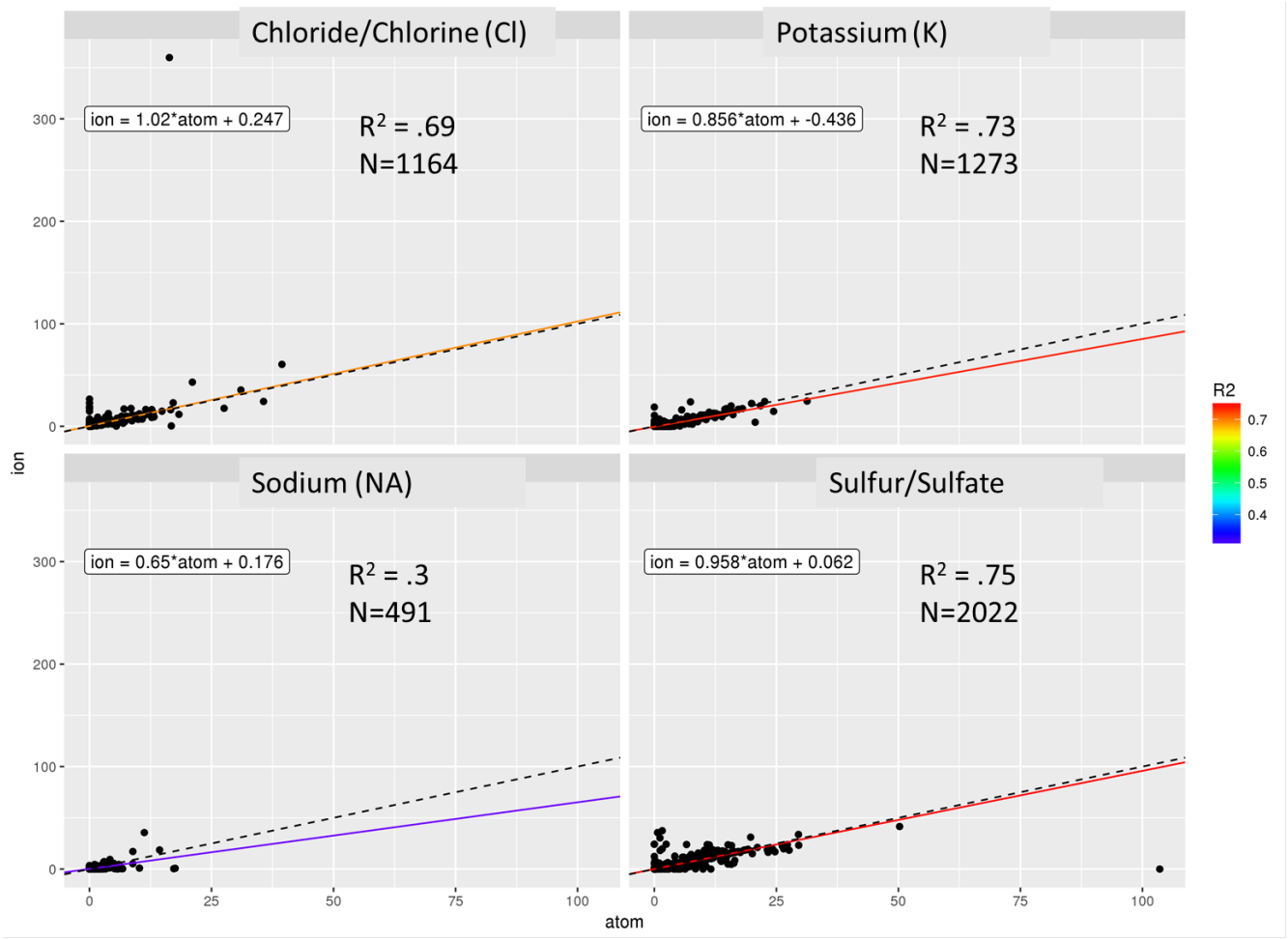
Table G-1 shows the AE6 species used in CMAQ and how the species in the SPECIATE database maps to each of them. This mapping uses the Speciation Tool to create the SMOKE-ready speciation profiles. The comments column indicates which species are typically not found in the literature and thus need to be computed by this protocol. These species are PNCOM and PH20. The comments also describe the gap filling procedures for when the exact species ID is not present in the profile, but a different form (i.e., atomic vs ionic) of the pollutant is available. Gap filling procedures are provided for sodium (Na), magnesium (Mg), chlorine (Cl), calcium (Ca), potassium (K) and sulfate (S). In some studies, the atomic form is measured but not the ionic form. The atomic form results from the use of x-ray fluorescence (XRF) as the measurement technique and the ionic form results from the use of ion chromatography. Gap filling is needed because the study may have measured only the atomic form of the metal, but the model uses the ionic form. Rather than putting in a 0 for the ionic form, the weight percent of the atomic form is used. Some profiles have both atomic and ionic forms and when doing a regression, we found that other than Na which has a poor regression coefficient, the weight percents of the ion/atomic forms closely follow each other (see Figure G-1). Note that Mg and Ca did not have sufficient data points for a meaningful regression and are not shown. Finally, the comments in Table G-1 indicate if there were changes made to the mapping from version 4.2 of the Speciation Tool. The changes to the mapping from version 4.2 of the Speciation Tool are made because for CMAQ, the AE6 uses the ionic form of several metals whereas version 4.2 assigned the atomic form.

Table G-1: PM Model Species: AE6

Species Name	Species ID	Species Description, Chemical Formula	Comments/Updated Mappings From
POC	626	Organic carbon	This is obtained from the measurement study, but the weight percent may need to be adjusted downward when creating an AE6 profile if the sum of the species' weight percents exceed 100. The adjustment assumes that the POC included measurement artifacts and is adjusted to achieve mass conservation.
PEC	797	Elemental carbon	
PSO4	699	Sulfate, SO_4^{2-}	Gap filling procedure: If the profile has sulfur (species ID = 700) but no sulfate, then compute sulfate stoichiometrically (SO_4^{2-}=96/32*S)
PNO3	613	Nitrate, NO_3^-	
PNH4	784	Ammonium, NH_4^+	
PNCOM	2669	non-carbon organic matter	Computed from OC based on the (OM to OC ratio) which is a function of the source characteristics and is based on the Reff et. al. (2009) default assignments: Mobile exhaust (combustion): 1.25 Wood combustion sources except wood fired boilers: 1.7 All other sources including wood fired boilers: 1.4 If a particular study uses a different ratio than the default (e.g., the Kansas City study profiles use 1.2 instead of 1.25), then that ratio would be used in place of the default.
PFE	488	Iron	
PAL	292	Aluminum	
PSI	694	Silicon	
PTI	715	Titanium	

Species Name	Species ID	Species Description, Chemical Formula	Comments/Updated Mappings From
PCA	2303	Calcium ion Ca^{2+}	This is a change from the Speciation Tool version 4.0 which used the atom (329). Gap filling procedure: If Species ID 2303 isn't present and Calcium (Species ID 329) is present, then use Species ID 329. If neither Species ID 2303 nor Species ID 329 are present but calcium oxide (CaO Species ID 2847) is present, then Ca^{2+} = 40/56* CaO.
PMG	2772	Magnesium ion Mg^{2+}	This is a change from the Speciation Tool version 4.0 which used the Magnesium atom (Species ID 525). Gap filling procedure: If Species ID 2772 isn't present and Magnesium atom (Species ID 525) is present, then use Species ID 525. If neither Species ID 2772 nor Species ID 525 are present but Magnesium Oxide, MgO (2852) is present, then Mg^{2+}= 24/40* MgO
PK	2302	Potassium ion K^{+}	This is a change from the Speciation Tool version 4.0 which used the Potassium atom (Species ID 669). Gap filling procedure: If Species ID 2302 isn't present and Potassium atom (Species ID 669) is present, then use Potassium atom (Species ID 669).
PMN	526	Manganese	
PNA	785	Sodium ion Na^{+}	This is a change from the Speciation Tool version 4.0 which used the Sodium atom (Species ID 696). Gap filling procedure: If Sodium ion (Species ID 785) isn't present and Sodium atom (Species ID 696) is present, then use Sodium atom (Species ID 696).
PCL	337	Chloride ion	This is a change from the Speciation Tool version 4.0 which used the Chloride atom (Species ID 795). Gap filling procedure: If Chloride ion (Species ID 337) isn't present and Chlorine atom (Species ID 795) is present, then use Chlorine atom (Species ID 795).
PH2O	2668	Water	Computed for non-combustion and non-high temperature sources
PMO	2671	$PM_{2.5}$ not in other AE6 species	Optional for PM-AE6 profile in SPECIATE but computed in the Speciation Tool. (can compute or leave out). Computed from 100-sum of other species.

Figure G-1. Regression of Ion and Atom Forms for Profiles which Contain Data for Both



The comments column also indicates gap filling techniques to use if the measurements from the literature are in a different form (i.e., atomic instead of ionic) than the AE6 species. Also, POC and PNCOM species may need to be adjusted from the values in the paper. Adjustment of these may be needed to account for artifacts on the organic carbon (OC) measurement, or when the sum of weight percent across all unique species exceeds 100%. It should be noted that in order for a profile to be used in air quality modeling using the AE6 mechanism, it must have either PH2O or PNCOM. This is a requirement of the Speciation Tool which prepares the PM-AE6 speciation profiles in SPECIATE for SMOKE.

Instructions for Creating AE6 Profiles for Inclusion in SPECIATE

Step 1 – Read the reference (i.e., paper or report) and supplemental information carefully to get the mass fraction information, and determine if some species should not be included due to comments in the paper. Note the measurement methods (can be different for different species), whether the source is controlled, and if so using what measures.

Step 2: Map species in the reference to SPECIATE species and assign Species IDs

Step 3: Determine if OC needs to be adjusted due to "artifacts."

Artifacts are volatiles that condense in the sampler. These should not be counted as PM because they are in the gas phase and are not emitted from the source as condensed PM.

We believe that a non-zero back up filter measurement does provide evidence for positive artifacts and *may* be able to be quantitatively used to adjust by subtracting the backup from the primary filter. However, if the two filters provide similar values, and the difference results in very small OC with high uncertainty, then that difference value should not be quantitatively used to estimate "true" OC because of the high uncertainty. It is possible that some of the mass on the back-up could be mass desorbed from the primary filter.

If a quantitative estimate of "true" OC or an adjustment to compute it is provided in the paper, then use this to adjust OC. If neither are available from the paper, a judgement should be made on a case-by-case basis on whether or not to estimate "true" OC as the difference between the primary and secondary filter measurements. The guidance here is that if the primary filter and back up filter measurements are close, then it is not appropriate to use the difference (a very small number) as the "true" OC.

If there is no adjustment provided or is too uncertain (masses of primary and secondary are similar), and there appear to be artifacts, then OC can be adjusted later if the mass exceeds 100% after adding in the other AE6 species that are not contained in the paper.

Step 4: ADD particulate water, PH20. Note that this is SPECIES ID 2668 in SPECIATE.

The approach here is from the supplemental information from Reff, et. al, section S3.7.1

Type of Source	Particulate Water (PH2O) calculation
Combustion and other high temperature sources, where water is likely to be emitted in the vapor phase	0
All other sources	24% of the sum of sulfate (PSO4) and ammonium (PNH4) concentrations or percentages

Sources for which we assume 0 PH2O emissions are:

Agricultural Burning, Bituminous Combustion, Calcium Carbide Furnace, Charbroiling, Charcoal Manufacturing, Distillate Oil Combustion, Electric Arc Furnace, Ferromanganese Furnace, Glass Furnace, HDDV Exhaust, Heat Treating, Kraft Recovery Furnace, LDDV Exhaust, Lignite Combustion, Lime Kiln, Meat Frying, Natural Gas Combustion, Nonroad Gasoline Exhaust, Onroad 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 Boiler.

Step 5: For ammonium sulfate production or ammonium nitrate production: Add ammonium per Reff et. al. Section 3.7.4. These are imputed stoichiometrically assuming $(NH_4)_2SO_4$ for ammonium sulfate production and NH_4NO_3 for ammonium nitrate production.

If ammonium is computed, document it in the NOTES field of the SPECIATE database.

Step 6: Make sure there is consistency in sulfate and sulfur. If a profile has sulfate and not sulfur, the sulfur does not need to be computed, but if it has sulfur but not sulfate it should be computed as follows:

$$SO_4 = \left(\frac{96}{32}\right) * S$$

If sulfate is computed document in the NOTES field of the SPECIATE database.

Step 7: Add Metal Bound Oxygen, MO. Note that this is SPECIES ID 2670 in SPECIATE.

While MO is not an AE6 species, it needs to be computed and included in the profile (unless it is 0) to enable a check for total mass fraction <= 100%.

The approach to compute MO follows Section S.3.7.2 in from Reff, et. al., which is to stoichiometrically combine oxygen with the metals, and then adjust the MO downward based on the amount of available sulfate in the profile. This approach assumes that the sulfates bind to the metals preferentially over the oxygen. A change from the Reff, et. al., approach is to use only the difference between the atomic and ionic masses for Na, Ca, Mg and K since the ionic version would not be the portion bound to oxygen.

Unadjusted MO is computed as

$$\boldsymbol{MO_{unadjusted} = \sum_{El}^{N} Ox_{El} \times E_{El}} \quad (1)$$

where Ox_{El} is the oxygen-to-metal ratio for metal El (Table 3), and E_{El} is the emission of metal El, **except for Na, Ca, Mg and K**. For these 4 metals, the E_{El} should reflect the difference between the atom form of the metal and the ion form. If, for Na, Ca, Mg, and K, the profile has only one form (atom or ion but not both) then the E_{El} should be set to 0. Also if the difference is negative, it should be set to 0.

Note that for metals in which there are multiple forms of the MO compound, an average of the oxygen to metal ratios across all forms is used.

To adjust MO based on preferential combining of sulfate over oxygen, compute the available sulfate for binding with metals, which is the sulfate remaining after fully neutralizing the NH_4^+ in the profile.

$$\boldsymbol{Neutralized\ SO_4^{2-} = \frac{0.5 * 96}{18} \times E_{NH_4^+}} \quad (2)$$

Where $E_{NH_4^+}$ is the mass of NH_4^+ in the profile.

The non-neutralized sulfate is the remainder from the sulfate in the profile.

$$\boldsymbol{Non\_Neutralized\_SO_4^{2-} = E_{SO_4^{2-}} - Neutralized\ SO_4^{2-}} \quad (3)$$

If $Non\_Neutralized\ SO_4^{2-} < 0$,

$$\boldsymbol{MO_{adjusted} = MO_{unadjusted}} \quad (4)$$

If $Non\_Neutralized\ SO_4^{2-} > 0$

$$\boldsymbol{MO_{adjusted} = MO_{unadjusted} - Non\_Neutralized\ SO_4^{2-} \times \frac{16}{96}} \quad (5)$$

$$\boldsymbol{If\ MO_{adjusted} < 0,\ MO_{adjusted} = 0} \quad (6)$$

If the difference is >0 between atom and ion for NA, Ca, Mg, and K, use that for the MO calculation. Otherwise set the MO for these metals to 0.

Table G-2: Assumed Oxide Forms of Each Metal and Resulting Mean Oxygen-to-Metal Ratio Used in Equation 1

Species	MW of metal[1]	Oxide Form 1	Oxide Form 2	Oxide Form 3	Oxygen/Metal Ratio
Na (Use difference between atom and ion)	22.99	Na_2O			0.348
Mg(Use difference between atom and ion)	24.31	MgO			0.658
Al	26.98	Al_2O_3			0.889
Si	28.09	SiO_2			1.139
P	30.97	P_2O_3	P_2O_5		1.033
K(Use difference between atom and ion)	39.10	K_2O			0.205
Ca(Use difference between atom and ion)	40.08	CaO			0.399
Ti	47.87	TiO2			0.669
V	50.94	V_2O_5			0.785
Cr	52.00	Cr_2O_3	CrO_3		0.692
Mn	54.94	MnO	MnO_2	Mn_2O_7	0.631
Fe	55.85	FeO	Fe_2O_3		0.358
Co	58.93	CoO	Co_2O_3		0.339
Ni	58.69	NiO			0.273
Cu	63.55	CuO			0.252
Zn	65.39	ZnO			0.245
Ga	69.72	Ga_2O_3			0.344
As	74.92	As_2O_3	As_2O_5		0.427
Se	78.96	SeO	SeO_2	SeO_3	0.405
Rb	85.47	Rb_2O			0.094
Sr	87.62	SrO			0.183
Zr	91.22	ZrO_2			0.351
Mo	95.94	MoO_2	MoO_3		0.417
Pd	106.42	PdO	PdO_2		0.226
Ag	107.87	Ag_2O			0.074
Cd	112.41	CdO			0.142
In	114.82	In_2O_3			0.209
Sn	118.71	SnO	SnO_2		0.202
Sb	121.76	Sb_2O_3	Sb_2O_5		0.263
Ba	137.33	BaO			0.117
La	138.91	La_2O_3			0.173
Ce	140.12	Ce_2O_3	CeO_2		0.200
Hg	200.59	Hg2O	HgO		0.060
Pb	207.20	PbO	PbO_2		0.116

Step 8: Add particulate non-carbon organic matter (PNCOM)

Every profile that has POC must have PNCOM computed from POC. If the paper (also check the Supplemental information) provides a factor to compute this, use the value provided in the paper. Otherwise, use the default values provided in section S.3.7.3 of Reff, et, al. These values are provided in the box below. Populate the ORGANIC_MATTER_to_ORGANIC_CARBON_RATIO field in SPECIATE as 1 plus the fraction used (e.g., the default values are provided in the table below). Also, indicate in the NOTES field of the SPECIATE database how PNCOM was computed.

Type of Source	Computation of PNCOM	ORGANIC_MATTER_ to_ORGANIC_CARBON _RATIO
Onroad and Nonroad motor vehicle exhaust profiles (e.g., the HDDV Exhaust, Nonroad Gasoline Exhaust, Onroad Gasoline Exhaust, and LDDV Exhaust source categories):	$PNCOM = 0.25 * POC$	1.25
Wood combustion sources other than wood-fired boilers (e.g., wildfires, agricultural burning, residential wood combustion, prescribed burning, slash burning	$PNCOM = 0.7 * POC$	1.7
Wood-fired boilers and ALL OTHER SOURCES	$PNCOM = 0.4 * POC$	1.4

Step 9: Check for sum of $PM_{2.5}$ weight fractions over 100%

No adjustments need to be made if the weight fraction is less than 101%.

In this check, Sulfur should be excluded because it is double counted with sulfate. If the mass is still over 100% then:

1) Double check the paper to see if there are POC artifacts. If so and there is no quantitative information in the paper, **then adjust POC and PNCOM down by the same multiplier until the sum of weight fractions is 100%**
2) If POC artifacts have already been corrected for, there is not likely to be POC artifacts or POC is already very low and adjusting it would not reduce the total to 100%, then adjust all species down (i.e., normalize all weight percents) to get the sum to be 100%. If any of these adjustments are made, it should be documented in the NOTES.