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# SPECIATE 4.3: ADDENDUM TO SPECIATE 4.2

## SPECIATION DATABASE DEVELOPMENT DOCUMENTATION

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# ABSTRACT

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

The purpose of this addendum is to document how EPA developed the SPECIATE 4.3 database that updates the prior version of the SPECIATE 4.2 database. The majority of 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, pulp and paper industry, and several other stationary sources. In total, there were 151volatile organic gas profiles, 244 PM profiles, and 10 speciated mercury profiles appended to the SPECIATE 4.3 database. The SPECIATE 4.3 database includes a total of 5,592 PM, volatile organic gases, and Other Gases profiles.

# ACKNOWLEDGMENTS

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- EPA Office of Transportation and Air Quality (OTAQ) – Joseph Somers
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# Section I. Introduction

SPECIATE is the U.S. EPA repository of volatile organic gas and particulate matter (PM) speciation profiles of air pollution sources. Among the many uses of speciation data, these emission profiles may be used to: (1) create speciated emissions inventories for regional haze, PM, greenhouse gas (GHG), and photochemical air quality modeling; (2) estimate hazardous air pollutant (HAP) and toxic air pollutant (TAP) emissions from PM and organic gas primary emissions; (3) provide input to the Chemical Mass Balance (CMB) receptor model; and, (4) verify profiles derived from ambient measurements by multivariate receptor models (e.g., factor analysis and positive matrix factorization).

The SPECIATE 3.2 database that was released in 2002 contains profiles that are the result of testing and/or studies that were conducted in the 1980s, and in some cases, the 1970s. However, there are numerous sources of speciation data for PM, volatile organic compounds (VOC), and total organic gases (TOG, which include non-VOC) available from recent research studies and air quality management agency surveys. The EPA has been collecting new speciation data and collaborating with researchers to update the SPECIATE database. As a result, EPA released an updated SPECIATE database version 4.0 and database development documentation (EPA, 2006). Since the release of SPECIATE 4.0, there have been numerous new profiles added to the databases, which are named SPECIATE 4.1, 4.2, and 4.3. The purpose of this report is to summarize recent updates made to the latest SPECIATE 4.3 database. Copies of the updated database described in this report can be obtained online at http://www.epa.gov/ttn/chief/software/speciate/ or from the EPA Work Assignment Manager, Mr. Lee Beck (Beck.Lee@epa.gov). The reader is encouraged to visit this web presentation for access to complete documentation, downloadable versions of the SPECIATE database, access to the SPECIATE Data Browser, and other useful information associated with SPECIATE.

This report documents the development of the SPECIATE 4.3 database, which updates the SPECIATE 4.2 database. SPECIATE 4.3 includes a total of 5,592 profiles (with 5,187 carried forward from SPECIATE 4.2). Therewere 151volatile organic gasprofiles,244 PM profiles, and 10 speciated mercury profiles appended to this version of the database. For detailed documentation of the SPECIATE database (e.g., structure, source profile preparation methods), please refer to the SPECIATE 4.2 Database Development Documentation (EPA, 2009).

The SPECIATE user community has a wide range of interests and needs. Receptor modelers use SPECIATE as a source of data for emission source chemical profiles. Photochemical modelers make use of speciation data to properly characterize photochemical reactivity of VOC emissions and the chemical composition of PM emissions. Emission inventory preparers often turn to SPECIATE to fill data gaps in inventories of TAPs (which include HAPs) and GHG (e.g., methane, or black carbon reported as elemental carbon). Also, air quality control strategy analysts have an interest in the chemical make-up of VOC and PM emissions, so that control programs can better target the appropriate sources.

The steering committee for this project is a working group of EPA and E.H. Pechan & Associates, Inc. (Pechan) staff, university researchers, receptor/photochemical/dispersion modelers, emission inventory developers, and government agency staff. Members of the

workgroup have contributed and/or gathered data, and have provided recommendations as to which specific speciation profiles should be added to the database.

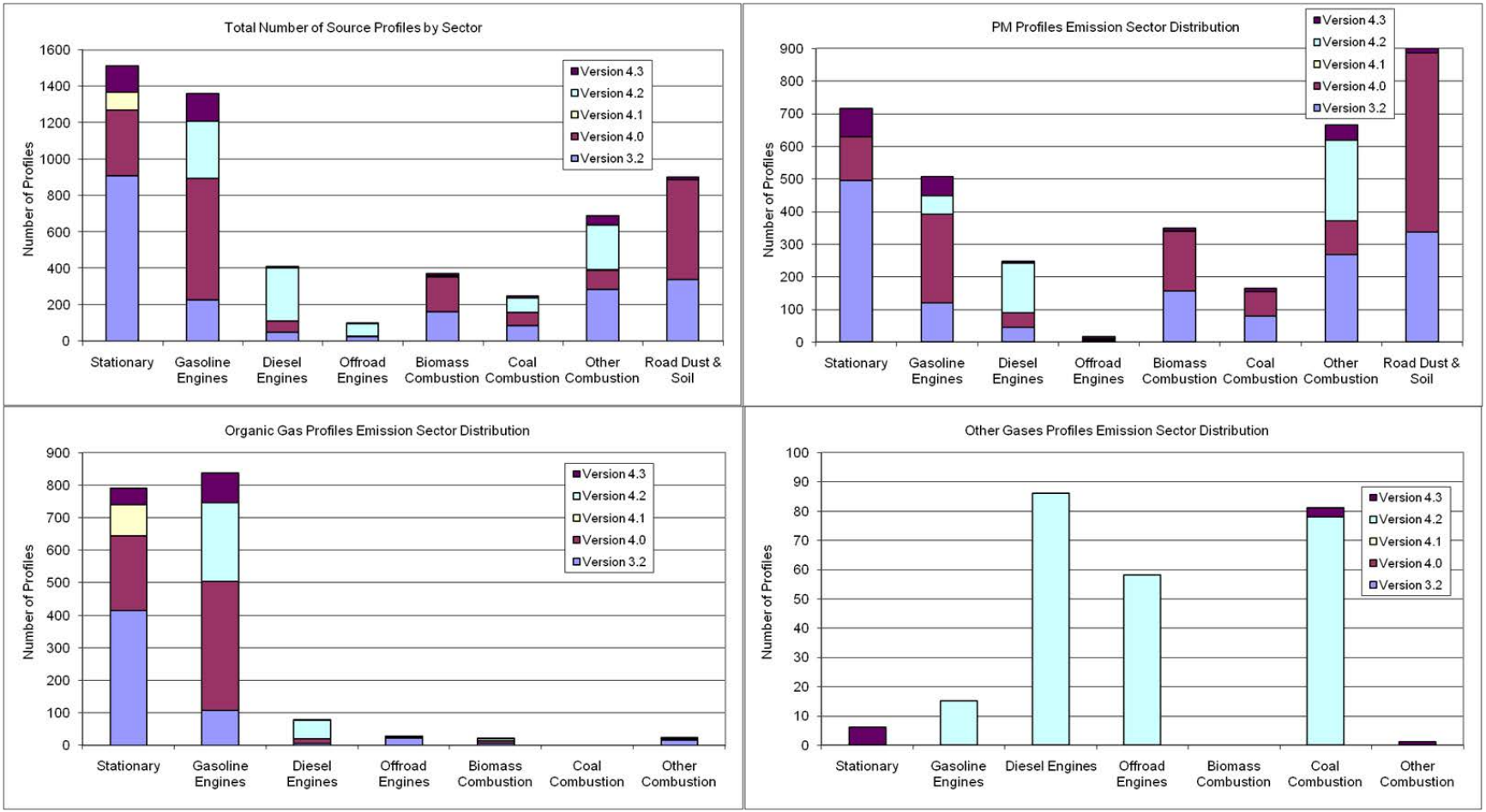
The primary purpose of this project was to update the most recent SPECIATE database to capture recent and scientifically-meritorious volatile organic gases and PM speciation profile data available from EPA, state agencies, peer-reviewed literature and other relevant data sources. SPECIATE 4.3 allows for storage of important information underlying each profile (meta data such as sampling and analysis methods, overall subjective profile quality ratings, etc.). In addition, ancillary data are also updated. These include the VOC-to-TOG conversion factors and the SCC-to-SPECIATE profile cross-reference table.

To date and as shown in Figure 1, the initiative to update SPECIATE has produced:

- 3,570 PM profiles;
- 1,775 volatile organic gas profiles;
- 247 Other Gases profiles;
- A total of 2,274 unique species;

While the database has been revised and many profiles have been added, the SPECIATE workgroup has identified and prioritized many data sets for which profiles will be developed and added to future versions of the SPECIATE database as resources allow.

**Figure 1. Number of Source Profiles by Profile Type, Source Sector, and SPECIATE Version**



## Section II. New Profiles in SPECIATE 4.3 Database

Lists of thenew profiles appended to the SPECIATE 4.3 database areprovided and described in this section. Tables 1 and 2 include new organic gas and PM profiles incorporated into the SPECIATE 4.3 database, respectively. Table 3 lists 10 new speciated mercury profiles added to this version of database. Finally, Table 4 presents a list of new chemical species as a result of incorporating new profiles into the SPECIATE 4.3 database.

The new profiles added to the SPECIATE 4.3 version are based on recent recommendations from the SPECIATE workgroup. One of the major data sources for this update is the EPA Office of Transportation and Air Quality (OTAQ). The EPA OTAQ has conducted several large emission characterization studies which produced many comprehensive speciation data sets. For example, the Kansas City PM Characterization Study (EPA 2008) tested over 50 light duty gasoline vehicles for both PM and non-methane organic gas (NMOG) emissions. Speciation profiles based on these individual tests are incorporated into the current version of the SPECIATE database. Since they are in the same vehicle category, they all share the same profile name. Multiple TOG speciation profiles which characterize gasoline engine exhaust fueled with three ethanol blends were also supplied by EPA OTAQ. Another important TOG emission sector studied was the diurnal permeation evaporative emissions. These TOG speciation profiles are based on three ethanol blends at 2 different Reid Vapor Pressures (RVPs). All of these profiles have been adapted for air quality modeling and policy making consideration (OTAQ, 2010).

SPECIATE 4.3 includes emission profiles for internal combustion engine exhaust from marine vessels using heavy oil and onroad vehicles based on liquefied petroleum gas, ethanol fuel production industry, oil-fired boilers, residential wood combustion, landfill gas, olefin manufacturing, and petroleum refining industry. In addition, there are 44 non-methane organic gas and PM profiles added to characterize the pulp and paper industry emissions. Speciation data corresponding to all sources pertinent to kraft, sulfite and non-chemical pulp mills, including bleach plants, pulping and repulping area sources, kraft and sulfite chemical recovery, paper machines wood residue, bark-fired boilers, and combination boilers firing various fuels. These pulp and paper industry speciated emissions data were mainly compiled from EPA, California, and Texas sponsored studies.

One hundred and seventy new composite and simplified PM profiles are also incorporated. They are based on a peer reviewed journal article published by several of the SPECIATE workgroup members (Reff et al., 2009). The authors carefully filtered through emission profiles in SPECIATE and selected individual profiles that represent a certain emission sector. The median of weight percents were calculated and renormalized to develop a composite profile. These composite PM profiles encompass a wide range of major emission sectors, including road dust, wildfires, agricultural burning, engine and fuel combustion exhaust, cement and other manufacturing industry, commercial cooking, etc. These profiles have been adapted for air quality modeling studies.

## Section III. Recommended Future Work

Recommended future tasks to further improve SPECIATE are:

1. Review and Update the "Source Classification Code (SCC)-to-Profile" Cross Reference Tables: The SCC-to-Profile tables include thousands of SCC codes and assigned speciation profiles for PM and organic gas emissions (EPA, 2010). These tables are essential for air quality modeling and toxic/speciated emission inventories. Some of the new profiles have been adapted and updated by EPA air quality modelers, e.g., new motor vehicle speciation profiles provided by EPA OTAQ. While the EPA's OAQPS posts SCC-to-profile cross-references formatted for the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system that used in their air quality modeling platforms (e.g., see www.epa.gov/ttn/chief/emch), they may not have all of the latest available profiles and they include only the SCCs in the inventories for the modeling platform. There are many other profiles available to better characterize emission compositions, e.g., pulp and paper industry, landfill gas, olefin manufacturing, and petroleum refining industry, etc. It is recommended that the project team review the SCC-to-Profile cross reference tables and identify outdated profiles. In addition to updating SCC-to-Profile cross reference tables with new profiles, this recommended review can be very helpful to identify future speciation data needs and update considerations.

2. Further Speciation Data Needs and Profile Development Prioritization: Based on the findings from reviewing the SCC-to-Profile cross reference tables, data search efforts should focus on source sectors that lack appropriate speciation profiles and where the emissions are significant. In addition, the workgroup has identified a long list of available speciation data sets. The findings from recommendation 1 should be considered to prioritize the future profile needs.

3. Develop Composite Profiles: There are many new profiles in the SPECIATE database that are based on individual tests. For example, the Kansas City PM Characterization Study (EPA, 2008) tested over 50 light duty gasoline vehicles for both PM and NMOG emissions. It is well known that emission compositions can vary significantly. Representative composite profiles are needed for source sectors that have multiple profiles available. It is recommended that users follow the Reff et al., (2009) methodology to carefully study these profiles and develop composite profiles.

## Section IV. References

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## Table 1. Summary of New Organic Gas Profiles Appended to SPECIATE 4.3 Database

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 5618 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S1-1 | NMOG | Individual test |
| 5619 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S1-2 | NMOG | Individual test |
| 5620 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-1 | NMOG | Individual test |
| 5621 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-2 | NMOG | Individual test |
| 5622 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-3 | NMOG | Individual test |
| 5623 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-4 | NMOG | Individual test |
| 5624 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S3-1 | NMOG | Individual test |
| 5625 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S3-2 | NMOG | Individual test |
| 5626 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S4-1 | NMOG | Individual test |
| 5627 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S4-2 | NMOG | Individual test |
| 5628 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-1 | NMOG | Individual test |
| 5629 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-2 | NMOG | Individual test |
| 5630 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-3 | NMOG | Individual test |
| 5631 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-4 | NMOG | Individual test |
| 5632 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-5 | NMOG | Individual test |
| 5633 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-1 | NMOG | Individual test |
| 5634 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-2 | NMOG | Individual test |
| 5635 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-3 | NMOG | Individual test |
| 5636 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-4 | NMOG | Individual test |
| 5637 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-1 | NMOG | Individual test |
| 5638 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-2 | NMOG | Individual test |
| 5639 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-3 | NMOG | Individual test |
| 5640 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-4 | NMOG | Individual test |
| 5641 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-1 | NMOG | Individual test |
| 5642 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-2 | NMOG | Individual test |
| 5643 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-3 | NMOG | Individual test |
| 5645 | Residential Oil Boilers | VOC | |
| 5647 | Residual Oil-Fired Power Plant | VOC | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 5649 | Kraft Process Recovery Boiler | NMOG | |
| 5650 | Residential Wood Combustion | NMHC | |
| 5651 | Landfill Gas - composite of extraction well gas | TOG | |
| 5652 | Landfill Gas - gas collection systems | NMOG | |
| 5653 | Landfill Gas - passive vents | NMOG | |
| 5654 | Landfill Gas - flux chamber samples | NMOG | |
| 5655 | Gasoline - Mobile Grade 87 - adjusted for oxygenates | TOG | |
| 5656 | Gasoline - Exxon Grade 87 - adjusted for oxygenates | TOG | |
| 5657 | Gasoline - Shell Grade 87 - adjusted for oxygenates | TOG | |
| 5658 | Gasoline - Mobile Grade 93 - adjusted for oxygenates | TOG | |
| 5659 | Gasoline - Exxon Grade 93 - adjusted for oxygenates | TOG | |
| 5660 | Gasoline - Shell Grade 93 - adjusted for oxygenates | TOG | |
| 5661 | Gasoline - Mobile Gasohol 85 - adjusted for oxygenates | TOG | |
| 5662 | Gasoline Headspace Vapor - Mobile Grade 87 - adjusted for oxygenates | TOG | |
| 5663 | Gasoline Headspace Vapor - Exxon Grade 87 - adjusted for oxygenates | TOG | |
| 5664 | Gasoline Headspace Vapor - Shell Grade 87 - adjusted for oxygenates | TOG | |
| 5665 | Gasoline Headspace Vapor - Mobile Grade 93 - adjusted for oxygenates | TOG | |
| 5666 | Gasoline Headspace Vapor - Exxon Grade 93 - adjusted for oxygenates | TOG | |
| 5667 | Gasoline Headspace Vapor - Shell Grade 93 - adjusted for oxygenates | TOG | |
| 5668 | Gasoline Headspace Vapor - Mobile Gasohol 85 - adjusted for oxygenates | TOG | |
| 5677 | Passenger ferry - four-stroke diesel engines | VOC | |
| 5678 | Passenger ferry - four-stroke diesel engines | VOC | |
| 8756 | Gasoline Exhaust - Tier 2 light-duty vehicles using 0% Ethanol - Composite Profile | TOG | |
| 8757 | Gasoline Exhaust - Tier 2 light-duty vehicles using 10% Ethanol - Composite Profile | TOG | |
| 8758 | Gasoline Exhaust - Tier 2 light-duty vehicles using 15% Ethanol - Composite Profile | TOG | |
| 8759 | Gasoline Exhaust - Cold Start - Tier 2 light-duty vehicles using 0% Ethanol - Composite Profile | TOG | |
| 8760 | Gasoline Exhaust - Cold Start - Tier 2 light-duty vehicles using 10% Ethanol - Composite Profile | TOG | |
| 8761 | Gasoline Exhaust - Cold Start - Tier 2 light-duty vehicles using 15% Ethanol - Composite Profile | TOG | |
| 8762 | Gasoline Headspace Vapor using 0% Ethanol - Composite Profile | TOG | |
| 8763 | Gasoline Headspace Vapor using 10% Ethanol - Composite Profile | TOG | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 8764 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 7 RVP - Composite Profile | TOG | |
| 8765 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 9 RVP - Composite Profile | TOG | |
| 8766 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol - Combined - Composite Profile | TOG | |
| 8767 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 7 RVP - Composite Profile | TOG | |
| 8768 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 10 RVP - Composite Profile | TOG | |
| 8769 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol - Combined - Composite Profile | TOG | |
| 8770 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 15% Ethanol - Combined | TOG | |
| 8771 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 7 RVP | TOG | |
| 8772 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 9 RVP | TOG | |
| 8773 | Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol - Combined | TOG | |
| 8774 | Diesel Exhaust Emissions from Pre-2007 Model Year Heavy-Duty Diesel Trucks | TOG | |
| 8775 | Diesel Exhaust Emissions from 2007 Model Year Heavy-Duty Diesel Engines with Controls | TOG | |
| 8776 | Dry Mill Fuel Ethanol Production - whole facility | TOG | |
| 8777 | Dry Mill Fuel Ethanol Production - cooling cyclone | TOG | |
| 8778 | Dry Mill Fuel Ethanol Production - distillation scrubber | TOG | |
| 8779 | Dry Mill Fuel Ethanol Production - fermentation bypass | TOG | |
| 8780 | Dry Mill Fuel Ethanol Production - fermentation scrubber | TOG | |
| 8781 | Dry Mill Fuel Ethanol Production - fluid bed cooler | TOG | |
| 8782 | Dry Mill Fuel Ethanol Production - thermal oxidizer | TOG | |
| 8783 | Pulp and Paper Mills - Kraft Mill Bleach Plants | NMOG | |
| 8784 | Pulp and Paper Mills - Kraft Oxygen Delignification System Vents | NMOG | |
| 8785 | Pulp and Paper Mills - Pulp Knotters | NMOG | |
| 8786 | Pulp and Paper Mills - Pulp Screens | NMOG | |
| 8787 | Pulp and Paper Mills - Vacuum Drum Type Brownstock Washers | NMOG | |
| 8788 | Pulp and Paper Mills - “Other” Brownstock Washers | NMOG | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 8789 | Pulp and Paper Mills - Kraft Pulp Deckers | NMOG | |
| 8790 | Pulp and Paper Mills - Batch Kraft Digester Relief Gases | NMOG | |
| 8791 | Pulp and Paper Mills - Continuous Kraft Digester Relief Gases | NMOG | |
| 8792 | Pulp and Paper Mills - Batch Kraft Digester Blow Gases | NMOG | |
| 8793 | Pulp and Paper Mills - Continuous Kraft Digester Blow Gases | NMOG | |
| 8794 | Pulp and Paper Mills - Batch Digester Kraft Pulp Mill Evaporator Gases | NMOG | |
| 8795 | Pulp and Paper Mills - Continuous Digester Kraft Pulp Mill Evaporator Gases | NMOG | |
| 8796 | Pulp and Paper Mills - Kraft Pulp Mill Stripper Gases | NMOG | |
| 8797 | Pulp and Paper Mills - Kraft Pulp Mill LVHC NCGs - Batch Digester and Evaporator Gases Only | NMOG | |
| 8798 | Pulp and Paper Mills - Kraft Pulp Mill LVHC NCGs - Continuous Digester and Evaporator Gases Only | NMOG | |
| 8799 | Pulp and Paper Mills - Kraft Batch Digester Fill Exhaust Gases | NMOG | |
| 8800 | Pulp and Paper Mills - Kraft NCG Thermal Oxidizers | NMOG | |
| 8801 | Pulp and Paper Mills - Weak Black Liquor Storage Tanks | NMOG | |
| 8802 | Pulp and Paper Mills - Strong Black Liquor Storage Tanks | NMOG | |
| 8803 | Pulp and Paper Mills - White and Green Liquor Storage Tanks | NMOG | |
| 8804 | Pulp and Paper Mills - Unbleached Kraft Pulp Storage Tanks | NMOG | |
| 8805 | Pulp and Paper Mills - Kraft Black Liquor Oxidation Tank Vents | NMOG | |
| 8806 | Pulp and Paper Mills - Kraft DCE Recovery Furnaces | NMOG | |
| 8807 | Pulp and Paper Mills - Kraft NDCE Recovery Furnaces | NMOG | |
| 8808 | Pulp and Paper Mills - Sulfite Recovery Furnaces | NMOG | |
| 8809 | Pulp and Paper Mills - Kraft Lime Kilns | NMOG | |
| 8810 | Pulp and Paper Mills - Kraft Smelt Dissolving Tanks | NMOG | |
| 8811 | Pulp and Paper Mills - Kraft Tall Oil Reactors | NMOG | |
| 8812 | Pulp and Paper Mills - Kraft Paper Machines and Pulp Dryers - Unbleached Linerboard Paper Machine | NMOG | |
| 8813 | Pulp and Paper Mills - Kraft Paper Machines and Pulp Dryers - Bleached Paper Machine & Pulp Dryer | NMOG | |
| 8814 | Pulp and Paper Mills - Wood-Fired Boilers | NMOG | |
| 8815 | Pulp and Paper Mills - Secondary Fiber Furnish Paper Machines | NMOG | |
| 8816 | Pulp and Paper Mills - Virgin Mechanical and Chemical Pulp Furnish Paper Machines | NMOG | |
| 8817 | Pulp and Paper Mills - Deinking (with Bleaching) Operations | NMOG | |
| 8818 | Pulp and Paper Mills - Mechanical Pulping Source Emissions - Thermomechanical Pulping | NMOG | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 8819 | Pulp and Paper Mills - Mechanical Pulping Source Emissions - Pressurized Groundwood | NMOG | |
| 8820 | Pulp and Paper Mills - Mechanical Pulping Source Emissions - Stone Groundwood | NMOG | |
| 8827 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 7 RVP | TOG | |
| 8828 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 9 RVP | TOG | |
| 8829 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol - Combined | TOG | |
| 8830 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 7 RVP | TOG | |
| 8831 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 9 RVP | TOG | |
| 8832 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol - Combined | TOG | |
| 8833 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 7 RVP | TOG | |
| 8834 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol at 9 RVP | TOG | |
| 8835 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 20% Ethanol - Combined | TOG | |
| 8836 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 7 RVP | TOG | |
| 8837 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 9 RVP | TOG | |
| 8838 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol - Combined | TOG | |
| 8839 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 7 RVP | TOG | |
| 8840 | 86°F  Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 10 RVP | TOG | |
| 8841 | 86°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol - Combined | TOG | |
| 8842 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 7 RVP | TOG | |
| 8843 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 9 RVP | TOG | |
| 8844 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol - Combined | TOG | |
| 8845 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 7 RVP | TOG | |
| 8846 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 10 RVP | TOG | |
| 8847 | 105°F Static Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol - Combined | TOG | |
| 8848 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 7 RVP | TOG | |
| 8849 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol at 9 RVP | TOG | |
| 8850 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol - Combined | TOG | |
| 8851 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 7 RVP | TOG | |
| 8852 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol at 10 RVP | TOG | |
| 8853 | Dynamic Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol - Combined | TOG | |
| 8854 | Gasoline Exhaust - Tier 2 light-duty vehicles using 20% Ethanol - Composite Profile | TOG | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 8855 | Gasoline Exhaust - Tier 2 light-duty vehicles using 85% Ethanol - Composite Profile | TOG | |
| 8856 | Liquefied Petroleum Gas (LPG) Composition | TOG | |
| 8857 | Light Duty Vehicle Exhaust - Liquefied Petroleum Gas (LPG) – Test ID 1 | TOG | |
| 8858 | Light Duty Vehicle Exhaust - Liquefied Petroleum Gas (LPG) – Test ID 2 | TOG | |
| 8859 | Light Duty Vehicle Exhaust - Liquefied Petroleum Gas (LPG) – Test ID 3 | TOG | |
| 8860 | Light Duty Vehicle Exhaust - Liquefied Petroleum Gas (LPG) – Average | TOG | |
| 8861 | Olefins manufacturing (ethylene and propylene, SIC 2869) – Composite Profile | VOC | |
| 8862 | Petroleum Refining (SIC 2911) - Composite Profile | VOC | |

Table 2. Summary of New PM Profiles Appended to SPECIATE 4.3 Database

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 5566 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S1-1 | PM | Individual test |
| 5567 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S1-2 | PM | Individual test |
| 5568 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-1 | PM | Individual test |
| 5569 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-2 | PM | Individual test |
| 5570 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-3 | PM | Individual test |
| 5571 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S2-4 | PM | Individual test |
| 5572 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S3-1 | PM | Individual test |
| 5573 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S3-2 | PM | Individual test |
| 5574 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S4-1 | PM | Individual test |
| 5575 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S4-2 | PM | Individual test |
| 5576 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-1 | PM | Individual test |
| 5577 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-2 | PM | Individual test |
| 5578 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-3 | PM | Individual test |
| 5579 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-4 | PM | Individual test |
| 5580 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S5-5 | PM | Individual test |
| 5581 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-1 | PM | Individual test |
| 5582 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-2 | PM | Individual test |
| 5583 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-3 | PM | Individual test |
| 5584 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S6-4 | PM | Individual test |
| 5585 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-1 | PM | Individual test |
| 5586 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-2 | PM | Individual test |
| 5587 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-3 | PM | Individual test |
| 5588 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S7-4 | PM | Individual test |
| 5589 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-1 | PM | Individual test |
| 5590 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-2 | PM | Individual test |
| 5591 | Light Duty Vehicle Exhaust - Gasoline - Test ID: S8-3 | PM | Individual test |
| 5592 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W1-1 | PM | Individual test |
| 5593 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W1-2 | PM | Individual test |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 5594 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W1-3 | PM | Individual test |
| 5595 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W2-1 | PM | Individual test |
| 5596 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W2-2 | PM | Individual test |
| 5597 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W2-3 | PM | Individual test |
| 5598 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W3-1 | PM | Individual test |
| 5599 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W3-2 | PM | Individual test |
| 5600 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W3-3 | PM | Individual test |
| 5601 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W4-1 | PM | Individual test |
| 5602 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W4-2 | PM | Individual test |
| 5603 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W4-3 | PM | Individual test |
| 5604 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W5-1 | PM | Individual test |
| 5605 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W5-2 | PM | Individual test |
| 5606 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W5-3 | PM | Individual test |
| 5607 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W6-1 | PM | Individual test |
| 5608 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W6-2 | PM | Individual test |
| 5609 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W6-3 | PM | Individual test |
| 5610 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W6-4 | PM | Individual test |
| 5611 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W7-1 | PM | Individual test |
| 5612 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W7-2 | PM | Individual test |
| 5613 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W7-3 | PM | Individual test |
| 5614 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W7-4 | PM | Individual test |
| 5615 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W8-1 | PM | Individual test |
| 5616 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W8-2 | PM | Individual test |
| 5617 | Light Duty Vehicle Exhaust - Gasoline - Test ID: W8-3 | PM | Individual test |
| 5644 | Residential Oil Boilers | PM | |
| 5646 | Residual Oil-Fired Power Plant | PM | |
| 5648 | Kraft Process Recovery Boiler | PM | |
| 5669 | Gas-Fired Boilers | PM | |
| 5670 | Gas-Fired Process Heaters | PM | |
| 5671 | Gas-Fired Combined Cycle and Cogeneration Plants | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 5672 | Oil-Fired Boilers | PM | |
| 5673 | Diesel Engines | PM | |
| 5674 | Marine Vessel - Main Engine - Heavy Fuel Oil | PM | |
| 5675 | Marine Vessel - Auxiliary Engine - Marine Gas Oil | PM | |
| 5676 | Marine Vessel - Auxiliary Boiler - Heavy Fuel Oil | PM | |
| 5679 | Diesel Exhaust - Heavy-heavy duty truck - 2007 model year | PM | |
| 5680 | Diesel Exhaust - Heavy-heavy duty truck - 2007 model year | PM | |
| 5681 | Marine Vessel - Main Propulsion Engine - Heavy Fuel Oil | PM | |
| 5682 | Bituminous Coal-Fired Power Plant | PM | |
| 5683 | Construction Dust | PM | |
| 8821 | Pulp and Paper Mills - Kraft DCE Recovery Furnaces | PM | |
| 8822 | Pulp and Paper Mills - Kraft NDCE Recovery Furnaces | PM | |
| 8823 | Pulp and Paper Mills - Sulfite Recovery Furnaces | PM | |
| 8824 | Pulp and Paper Mills - Kraft Lime Kilns with ESPs | PM | |
| 8825 | Pulp and Paper Mills - Kraft Lime Kilns with Wet Scrubbers | PM | |
| 8826 | Pulp and Paper Mills - Kraft Smelt Dissolving Tanks | PM | |
| 91100 | Unpaved Road Dust - Composite | PM | |
| 91101 | Agricultural Soil - Composite | PM | |
| 91102 | Wildfires - Composite | PM | |
| 91103 | Agricultural Burning - Composite | PM | |
| 91104 | Bituminous Combustion - Composite | PM | |
| 91105 | Residential Wood Combustion - Composite | PM | |
| 91106 | HDDV Exhaust - Composite | PM | |
| 91107 | Construction Dust - Composite | PM | |
| 91108 | Paved Road Dust - Composite | PM | |
| 91109 | Prescribed Burning - Composite | PM | |
| 91110 | Sub-Bituminous Combustion - Composite | PM | |
| 91111 | Sand & Gravel - Composite | PM | |
| 91112 | Natural Gas Combustion - Composite | PM | |
| 91113 | Nonroad Gasoline Exhaust - Composite | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 91114 | Wood Fired Boiler - Composite | PM | |
| 91115 | Distillate Oil Combustion - Composite | PM | |
| 91116 | Charbroiling - Composite | PM | |
| 91117 | Residual Oil Combustion - Composite | PM | |
| 91118 | Dairy Soil - Composite | PM | |
| 91119 | Kraft Recovery Furnace - Composite | PM | |
| 91120 | Mineral Products - Avg - Composite | PM | |
| 91121 | Industrial Manufacturing - Avg - Composite | PM | |
| 91122 | Onroad Gasoline Exhaust - Composite | PM | |
| 91123 | Heat Treating - Composite | PM | |
| 91124 | Chemical Manufacturing - Avg - Composite | PM | |
| 91125 | Lignite Combustion - Composite | PM | |
| 91126 | Solid Waste Combustion - Composite | PM | |
| 91127 | Cement Production - Composite | PM | |
| 91128 | Wood Products - Drying - Composite | PM | |
| 91129 | Surface Coating - Composite | PM | |
| 91130 | Food & Ag - Handling - Composite | PM | |
| 91131 | Wood Products-Sawing - Composite | PM | |
| 91132 | Aluminum Processing - Composite | PM | |
| 91133 | Open Hearth Furnace - Composite | PM | |
| 91134 | Brake Lining Dust - Composite | PM | |
| 91135 | Meat Frying - Composite | PM | |
| 91136 | Process Gas Combustion - Composite | PM | |
| 91137 | Aluminum Production - Composite | PM | |
| 91138 | Lime Kiln - Composite | PM | |
| 91139 | Sintering Furnace - Composite | PM | |
| 91140 | Charcoal Manufacturing - Composite | PM | |
| 91141 | Catalytic Cracking - Composite | PM | |
| 91142 | Fiberglass Manufacturing - Composite | PM | |
| 91143 | Glass Furnace - Composite | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 91144 | Pulp & Paper Mills - Composite | PM | |
| 91145 | Petroleum Industry - Avg - Composite | PM | |
| 91146 | Slash Burning - Composite | PM | |
| 91147 | Misc. Sources - Composite | PM | |
| 91148 | Asphalt Roofing - Composite | PM | |
| 91149 | Inorganic Chemical Manufacturing - Composite | PM | |
| 91150 | Tire Dust - Composite | PM | |
| 91151 | Ferromanganese Furnace - Composite | PM | |
| 91152 | Wood Products - Sanding - Composite | PM | |
| 91153 | Electric Arc Furnace - Composite | PM | |
| 91154 | Food & Ag-Drying - Composite | PM | |
| 91155 | Residential Coal Combustion - Composite | PM | |
| 91156 | Residential Natural Gas Combustion - Composite | PM | |
| 91157 | Cast Iron Cupola - Composite | PM | |
| 91158 | Copper Processing - Composite | PM | |
| 91159 | Asphalt Manufacturing - Composite | PM | |
| 91160 | Fly Ash - Composite | PM | |
| 91161 | Sandblast - Composite | PM | |
| 91162 | LDDV Exhaust - Composite | PM | |
| 91163 | Ammonium Nitrate Production - Composite | PM | |
| 91164 | Limestone Dust - Composite | PM | |
| 91165 | Phosphate Manufacturing - Composite | PM | |
| 91166 | Gypsum Manufacturing - Composite | PM | |
| 91167 | Urea Fertilizer - Composite | PM | |
| 91168 | Lead Processing - Composite | PM | |
| 91169 | Crustal Material - Composite | PM | |
| 91170 | Copper Production - Composite | PM | |
| 91171 | Brick Grinding and Screening - Composite | PM | |
| 91172 | Calcium Carbide Furnace - Composite | PM | |
| 91173 | Coke Calciner - Composite | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 91174 | Industrial Soil - Composite | PM | |
| 91175 | Potato Deep Frying - Composite | PM | |
| 91176 | Sea Salt - Composite | PM | |
| 91177 | Sludge Combustion - Composite | PM | |
| 91178 | Lead Production - Composite | PM | |
| 91179 | Steel Desulfurization - Composite | PM | |
| 91180 | Auto Body Shredding - Composite | PM | |
| 91181 | Ammonium Sulfate Production - Composite | PM | |
| 91182 | Inorganic Fertilizer - Composite | PM | |
| 91183 | Boric Acid Manufacturing - Composite | PM | |
| 92095 | Draft Bituminous Coal Combustion - Simplified | PM | |
| 92100 | Unpaved Road Dust - Simplified | PM | |
| 92101 | Agricultural Soil - Simplified | PM | |
| 92102 | Wildfires - Simplified | PM | |
| 92103 | Agricultural Burning - Simplified | PM | |
| 92104 | Bituminous Coal Combustion - Simplified | PM | |
| 92105 | Residential Wood Combustion - Simplified | PM | |
| 92106 | HDDV Exhaust - Simplified | PM | |
| 92107 | Construction Dust - Simplified | PM | |
| 92108 | Paved Road Dust - Simplified | PM | |
| 92109 | Prescribed Burning - Simplified | PM | |
| 92110 | Sub-Bituminous Combustion - Simplified | PM | |
| 92111 | Sand & Gravel - Simplified | PM | |
| 92112 | Natural Gas Combustion - Simplified | PM | |
| 92113 | Nonroad Gasoline Exhaust - Simplified | PM | |
| 92114 | Wood Fired Boiler - Simplified | PM | |
| 92115 | Distillate Oil Combustion - Simplified | PM | |
| 92116 | Charbroiling - Simplified | PM | |
| 92117 | Residual Oil Combustion - Simplified | PM | |
| 92118 | Dairy Soil - Simplified | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 92119 | Kraft Recovery Furnace - Simplified | PM | |
| 92120 | Mineral Products - Avg - Simplified | PM | |
| 92121 | Industrial Manufacturing - Avg - Simplified | PM | |
| 92122 | Onroad Gasoline Exhaust - Simplified | PM | |
| 92123 | Heat Treating - Simplified | PM | |
| 92124 | Chemical Manufacturing - Avg - Simplified | PM | |
| 92125 | Lignite Combustion - Simplified | PM | |
| 92126 | Solid Waste Combustion - Simplified | PM | |
| 92127 | Cement Production - Simplified | PM | |
| 92128 | Wood Products - Drying - Simplified | PM | |
| 92129 | Surface Coating - Simplified | PM | |
| 92130 | Food & Ag - Handling - Simplified | PM | |
| 92131 | Wood Products - Sawing - Simplified | PM | |
| 92132 | Aluminum Processing - Simplified | PM | |
| 92133 | Open Hearth Furnace - Simplified | PM | |
| 92134 | Brake Lining Dust - Simplified | PM | |
| 92135 | Meat Frying - Simplified | PM | |
| 92136 | Process Gas Combustion - Simplified | PM | |
| 92137 | Aluminum Production - Simplified | PM | |
| 92138 | Lime Kiln - Simplified | PM | |
| 92139 | Sintering Furnace - Simplified | PM | |
| 92140 | Charcoal Manufacturing - Simplified | PM | |
| 92141 | Catalytic Cracking - Simplified | PM | |
| 92142 | Fiberglass Manufacturing - Simplified | PM | |
| 92143 | Glass Furnace - Simplified | PM | |
| 92144 | Pulp & Paper Mills - Simplified | PM | |
| 92145 | Petroleum Industry - Avg - Simplified | PM | |
| 92146 | Slash Burning - Simplified | PM | |
| 92147 | Misc. Sources - Simplified | PM | |
| 92148 | Asphalt Roofing - Simplified | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 92149 | Inorganic Chemical Manufacturing - Simplified | PM | |
| 92150 | Tire Dust - Simplified | PM | |
| 92151 | Ferromanganese Furnace - Simplified | PM | |
| 92152 | Wood Products - Sanding - Simplified | PM | |
| 92153 | Electric Arc Furnace - Simplified | PM | |
| 92154 | Food & Ag-Drying - Simplified | PM | |
| 92155 | Residential Coal Combustion - Simplified | PM | |
| 92156 | Residential Natural Gas Combustion - Simplified | PM | |
| 92157 | Cast Iron Cupola - Simplified | PM | |
| 92158 | Copper Processing - Simplified | PM | |
| 92159 | Asphalt Manufacturing - Simplified | PM | |
| 92160 | Fly Ash - Simplified | PM | |
| 92161 | Sandblast - Simplified | PM | |
| 92162 | LDDV Exhaust - Simplified | PM | |
| 92163 | Ammonium Nitrate Production - Simplified | PM | |
| 92164 | Limestone Dust - Simplified | PM | |
| 92165 | Phosphate Manufacturing - Simplified | PM | |
| 92166 | Gypsum Manufacturing - Simplified | PM | |
| 92167 | Urea Fertilizer - Simplified | PM | |
| 92168 | Lead Processing - Simplified | PM | |
| 92169 | Crustal Material - Simplified | PM | |
| 92170 | Copper Production - Simplified | PM | |
| 92171 | Brick Grinding and Screening - Simplified | PM | |
| 92172 | Calcium Carbide Furnace - Simplified | PM | |
| 92173 | Coke Calciner - Simplified | PM | |
| 92174 | Industrial Soil - Simplified | PM | |
| 92175 | Potato Deep Frying - Simplified | PM | |
| 92176 | Sea Salt - Simplified | PM | |
| 92177 | Sludge Combustion - Simplified | PM | |
| 92178 | Lead Production - Simplified | PM | |

| Profile Number | Profile Name | Profile Type | Note |
|---|---|---|---|
| 92179 | Steel Desulfurization - Simplified | PM | |
| 92180 | Auto Body Shredding - Simplified | PM | |
| 92181 | Ammonium Sulfate Production - Simplified | PM | |
| 92182 | Inorganic Fertilizer - Simplified | PM | |
| 92183 | Boric Acid Manufacturing - Simplified | PM | |
| 92200 | Marine Vessel - Auxiliary Boiler - Heavy Fuel Oil - Simplified | PM | |

Table 3. Summary of New Speciated Mercury Profiles Appended to SPECIATE 4.3 Database

| Profile Number | Profile Name | Profile Type |
|---|---|---|
| 6318 | Bituminous Coal-Fired Power Plant | Speciated Mercury |
| 6327 | Waste Disposal | Speciated Mercury |
| 6319 | Coal Combustion - Power Plants | Speciated Mercury |
| 6320 | Coal Combustion - Residential Heat | Speciated Mercury |
| 6321 | Oil Combustion | Speciated Mercury |
| 6322 | Cement Production | Speciated Mercury |
| 6323 | Non-Ferrous Metals - Lead | Speciated Mercury |
| 6324 | Non-Ferrous Metals - Zinc | Speciated Mercury |
| 6325 | Pig and Iron | Speciated Mercury |
| 6326 | Caustic Soda | Speciated Mercury |

Table 4. Summary of New Chemical Species Appended to SPECIATE 4.3 Database

| Species ID | CAS Number | Chemical Name |
|---|---|---|
| 2663 | 14331-85-2 | Protactinium |
| 2664 | 7440-52-0 | Erbium |
| 2665 | 7440-06-4 | Platinum |
| 2666 | 1560-86-7 | 2-methylnonadecane |
| 2667 | 6418-45-7 | 3-methylnonadecane |
| 2668 | 7732-18-5 | Particulate Water |
| 2669 | | Non-Carbon Organic Matter (see Note 1 below) |
| 2670 | | Metal-bound Oxygen (see Note 2 below) |
| 2671 | | Other Unspeciated PM2.5 (see Note 3 below) |
| 2672 | 18540-29-9 | Chromium(VI) |
| 2673 | 1072-05-5; 2040-96-2 | 2,6-dimethylheptane, propylcyclopentane |
| 2674 | 13269-52-8; 1120-62-3 | Trans-3-hexene; 3-methylcyclopentene |
| 2675 | 2738-19-4; 7642-10-6 | 2-methyl-2-hexene; cis-3-heptene |
| 2676 | 3899-36-3; 14686-13-6 | 3-methyl-trans-3-hexene; Trans-2-heptene |
| 2677 | 591-49-1; 589-53-7 | 1-methylcyclohexene; 4-methylheptane |
| 2678 | 109-67-1; 503-17-3 | 1-pentene; 2-butyne |
| 2679 | 110-83-8; 589-34-4 | Cyclohexene; 3-methylhexane |
| 2680 | 107-39-1; 10574-37-5 | 2,4,4-trimethyl-1-pentene; 2,3-dimethyl-2-pentene |
| 2681 | 691-38-3; 107-83-5 | 4-methyl-cis-2-pentene; 2-methylpentane (isohexane) |
| 2682 | 3074-71-3; 3221-61-2 | 2,3-dimethylheptane; 2-methyloctane |
| 2683 | 2207-03-6; 624-29-3 | Trans-1,3-dimethylcyclohexane; Cis-1,4-dimethylcyclohexane |
| 2684 | 300-57-2 | Allylbenzene |
| 2685 | 2198-23-4 | 4-nonene |
| 2686 | 7439-88-5 | Iridium |
| 2687 | | Hydrated sulfate (see Note 4 below) |
| 2688 | 513-86-0 | 3-Hydroxy-2-butanone |
| 2689 | 513-85-9 | 2,3-Butanediol |
| 2690 | 98-01-1 | 2-Furancarboxaldehyde (or Furfural) |

| Species ID | CAS Number | Chemical Name |
|---|---|---|
| 2691 | 50-21-5 | Lactic acid |
| 2692 | 624-92-0 | Dimethyl Disulfide |
| 2693 | 156-59-2 | 1,2-Dichloroethene |
| 2694 | 88-06-2 | 2,4,6-Trichlorophenol |
| 2695 | 51-28-5 | 2,4-Dinitrophenol |
| 2696 | 121-14-2 | 2,4-Dinitrotoluene |
| 2697 | 88-75-5 | 2-Nitrophenol (o-Nitrophenol) |
| 2698 | 13466-78-9 | 3-Carene |
| 2699 | 534-52-1 | 4,6-Dinitro-o-cresol |
| 2700 | 100-02-7 | 4-Nitrophenol |
| 2701 | 39638-32-9 | Bis(2-chloroisopropyl) ether |
| 2702 | 95-57-8 | 2-Chlorophenol |
| 2703 | 2051-24-3 | Decachlorobiphenyl |
| 2704 | 25512-42-9 | Dichlorobiphenyl |
| 2705 | 117-84-0 | Di-n-octyl phthalate |
| 2706 | 35065-27-1 | 2,2',4,4',5,5'-Hexachlorobiphenyl |
| 2707 | 77-47-4 | Hexachlorocyclopentadiene |
| 2708 | 32598-14-4 | 2,3,3',4,4'-Pentachlorobiphenyl |
| 2709 | 87-86-5 | Pentachlorophenol |
| 2710 | 26914-33-0 | Tetrachlorobiphenyl |
| 2711 | 38444-78-9 | 2,2',3-Trichlorobiphenyl |
| 2712 | 99-85-4 | Gamma-Terpinene |
| 2713 | 110-71-4 | 1,2-Dimethoxyethane |
| 2714 | 13389-42-9; 6876-23-9 | Trans-2-octene; Trans-1,2-dimethylcyclohexane |

Note:

1. Non-Carbon Organic Matter is calculated for each source category by multiplying OC emissions by a source-category specific OM/OC (OM = organic matter) ratio to calculate an OM emission, and subtracting OC from OM. PNCOM = POC*(OM/OC Ratio - 1) where POC is from each profile and OM/OC ratio is based on the "Supporting information for: Emissions Inventory of PM2:5 Trace Elements across the United States", By Adam Reff, Prakash V. Bhave, Heather Simon, Thompson G. Pace,

George A.Pouliot, J. David Mobley, and Marc Houyoux (http://www.epa.gov/AMD/peer/products/Reff_ES&T2008_supportInfo.pdf), e.g., 1.25 for on/off-road motor vehicle exhaus, 1.7 for wood combustion, 1.4 for other sources including marine vessel engines.

2. Metal-bound oxygen (MO) is calculated 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. Calculation details provided in supporting information of Adam Reff, Prakash V. Bhave, Heather Simon, Thompson G. Pace, George A.Pouliot, J. David Mobley, and Marc Houyoux (http://www.epa.gov/AMD/peer/products/Reff_ES&T2008_supportInfo.pdf).
3. Other Unspeciated PM2.5 is calculated by subtracting the sum of speciated compounds in a profile from 100% of PM2.5 mass.
4. A ratio of 6.5 H2O molecules to a H2SO4 molecule is used to calculate hydrated sulfate, because it represents the lowest energy state for a sulfate water complex. (Comprehensive Simultaneous Shipboard and Airborne Characterization of Exhaust from a Modern Container Ship at Sea, Cocker, Murphy et al, ES&T, VOL. 43, NO. 13, 2009, pp. 4626-4640)