EPA's SPECIATE 4.4 Database - Development and Uses

Extended Abstract # 102

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INTRODUCTION

SPECIATE is the EPA's repository of TOG, PM, and Other Gases speciation profiles of air pollution sources. It includes weight fractions of both organic species and PM and provides data in consistent units. Species include metals, ions, elements, and organic and inorganic compounds. The Other Gases category contains speciated mercury, nitrogen oxides (NO_x), and semi-volatile organic compounds (SVOC), which do not fall into TOG or PM profile categories. The latest published version of SPECIATE, SPECIATE Version 4.4 (SPECIATE 4.4), includes 5,728 profiles for PM, TOG and Other Gases. SPECIATE is housed in a Microsoft Access® database and can link to models directly or by using a simple interface.

Data used to create these profiles are obtained from a variety of sources including peer-reviewed journal articles and emissions testing conducted primarily by the EPA. The original source of the data used in each profile is documented in the SPECIATE database. Because the data come from a variety of sources, their quality varies greatly. The SPECIATE database includes a quality indicator field that ranks the quality of specific profiles. However, there are numerous sources of speciation data for PM, volatile organic compounds (VOC), and TOG (which include non-VOCs) available from recent research studies and air quality management agency surveys. The EPA continually develops new speciation data and collaborates with researchers to update the SPECIATE database.

SPECIATE is an important foundational component for the development of emission inventories used in air quality management and demonstrating attainment of the National Ambient Air Quality Standards (NAAQS). In other words, one must accurately estimate anthropogenic and biogenic emission sources for an area in order to develop relevant and cost-effective emission control measures and correctly model NAAQS attainment demonstrations. MOVES2014, the onroad/nonroad emissions inventory model required for state implementation plan (SIP) development, directly incorporates speciation profiles. The weight fractions of individual volatile organic species are used in atmospheric chemistry mechanisms within air quality models to predict ozone concentrations in the atmosphere. The profiles of particulate matter (PM) species weight fractions are specific to particle size ranges and are used to support air quality modeling for PM and visibility. SPECIATE provides a repository of compounds searchable by source category and pollutant.

The use of detailed profiles in emission inventories and air quality models improves their accuracy and ultimately enhances the effectiveness of air quality management strategies. The source profiles in SPECIATE are used to: 1) create speciated emissions inventories for regional haze, PM, greenhouse gas, and photochemical air quality modeling; 2) estimate hazardous and toxic air pollutant emissions from total PM and total organic gas (TOG) primary emissions; 3) provide input to chemical mass balance (CMB) receptor models; and 4) verify profiles derived from ambient measurements using multivariate receptor models (e.g., factor analysis and positive matrix factorization). These applications require information on the individual species and compounds which comprise the volatile organics and PM mass. SPECIATE emission profiles also underpin the newest data set used by OAQPS to run its emission inventory and other models [the 2011 National Emissions Inventory (NEI) modeling platform]. Moreover, improvements to speciated emission inventories are tied in with EPA's ability to make more informed co-benefits decisions in a multi-pollutant framework.

SPECIATE 4.4 was developed collaboratively with Abt Associates in a cooperative effort involving EPA's Office of Research and Development (ORD) and Office of Air Quality Planning and Standards (OAQPS) in Research Triangle Park, NC, and EPA's Office of Transportation and Air Quality (OTAQ) in Ann Arbor, MI. Development of profiles for SPECIATE is guided by a 40-member workgroup using a database development protocol and spreadsheet. The spreadsheet is housed in a Microsoft Excel® workbook, "Master Evaluation of Profiles," and was created in 2004 as part of a protocol for expansion of the database. This tool summarizes the known publication and other resources that contain speciated emission profiles identified through extensive literature reviews and Workgroup recommendations. The information in this workbook includes EPA's prioritization of profiles to be added to SPECIATE and estimates the resources needed for their incorporation. It is a dynamic tool that shows changing priorities, profile development resource needs, and other database prioritization factors. EPA partners and State/local air agencies require SPECIATE to be a dynamic database to keep up with the latest emissions information.

SPECIATE, housed in a Microsoft Access® database, can link to models directly or by using a simple interface. This eliminates the need to enter the data manually and attendant potential for transposition errors. In addition to populating and maintaining the SPECIATE database itself, this effort also provides and maintains an online browser for researchers that do not have database proficiency but need information on the components of the emission profiles. The SPECIATE Web Browser is a web application developed to provide access through a simple web interface, allowing complex searches and downloads.

SPECIATE APPROACH AND ACCOMPLISHMENTS

The SPECIATE Workgroup

Given the importance of SPECIATE to the process of air quality management, an EPA SPECIATE Workgroup (Workgroup) was organized in 2004 to update SPECIATE. The Workgroup for this project consists of EPA and Abt Associates staff, university researchers, receptor/photochemical/dispersion modelers, emission inventory developers, and government

agency staff. Members of the Workgroup contribute and gather data, and provide recommendations as to which specific speciation profiles should be added to the database. SPECIATE users are typically individuals who: 1) conduct regional haze, fine PM, and ozone modeling; 2) prepare speciated emissions inventories; 3) use CMB or other receptor models; 4) and/or conduct chemically speciated, source-characterization experiments which expand the database.

The scope of work undertaken by the Workgroup is to: 1) update the SPECIATE database to capture recent and scientifically meritorious VOC, TOG, and PM speciation profile data available from EPA, state agencies, peer-reviewed literature, and other relevant data sources; 2) modify the structure of the SPECIATE database to allow for storage of important information underlying each profile (metadata such as sampling and analysis methods, overall subjective profile quality ratings); 3) link the new profiles to Source Classification Codes (SCCs) in the NEI; and 4) assign species to photochemical reactivity classes.

To address specific topics that arise during Workgroup meetings, Workgroup Committees are established. Presently, there are three Workgroup Committees exploring options to expand SPECIATE to include additional pertinent information: 1) the Black Carbon (BC) Committee that is investigating analytical methods to measure black carbon and whether scientifically meritorious data on black carbon exists and should be incorporated into speciation profiles; 2) the Maximum Incremental Reactivity (MIR) Committee that is investigating whether MIR values, used to evaluate impact on ozone production, should be incorporated into SPECIATE as a new data field; and 3) the Secondary Organic Aerosols (SOA) Committee that is evaluating SOA and brown carbon issues.

Nifty Bells and Whistles

SPECIATE has continuously evolved over its lifetime. Paper and computerized versions of SPECIATE were first available in 1988 for EPA applications. The first electronic version (CD) was distributed to the user community in 1993. SPECIATE 3.2 was posted to EPA's CHIEF website in 2002 as a front-end via desk top application. In 2007, Environment Canada provided data and resources to enhance and expand SPECIATE 4.1. The Other Gases category, SVOC Splitting Factors table, and Web Browser feature, were incorporated into SPECIATE 4.2, completed in 2009. SPECIATE 4.3 was completed in 2011 and completed the initial mapping of emission profiles to SCCs. It also added composite profiles for 58 (47 PM and 11 VOC) source categories. SPECIATE 4.3 mapped VOCs not previously in the SPECIATE database into model species commonly found in atmospheric chemical mechanisms[1].

SPECIATE Web Browser

The Web Browser is a web-based application to allow access to the SPECIATE database through a web interface[2]. This web-based application facilitates direct download of SPECIATE source profiles (i.e., Microsoft Access® is not needed). The application allows data searches by pollutant, keyword and category.

SVOC Splitting Factors

Since the release of SPECIATE 4.2, a new table has been included, titled "Semi-volatile Organic Compounds (SVOC) Splitting Factors." This table provides suggested SVOC partitioning factors in PM and gaseous phases[3]. Note that the partitioning factor of each SVOC species is not universal, but dependent on sampling conditions (e.g., temperature and pressure).

VOC-to-TOG Conversion Factors

Volatile organic compound (VOC) to total organic gas (TOG) conversion factors are provided for applicable gas profiles. The process of calculating the VOC-to-TOG conversion factor for a given profile consists of determining the organic gases in the profile that are exempted from the EPA definition of VOC and determining what portion of the overall profile is composed of these non-photochemically reactive compounds (e.g., methane, ethane, acetone).

SCC-to-SPECIATE Profile Cross-Reference Table

Since 2011, SPECIATE has mapped emission profiles to SCCs. SPECIATE 4.4 updated the SCC-to-SPECIATE profile cross-reference table to account for over 80% of national VOC and PM emissions in the NEI[4].

Highlights of SPECIATE 4.4

EPA released SPECIATE 4.4 and its documentation on February 28, 2014[4, 5]. It includes 5,728 PM, VOC, TOG, PM, and Other Gases profiles. SPECIATE 4.4 added 32 PM profiles for a total of 3,600; 104 TOG profiles for a total of 1,879; and 2,346 unique chemical species. The SPECIATE 4.4 database can be downloaded from the EPA website.

An enhancement to SPECIATE 4.4 is the comprehensive speciation of 40 new 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, outdoor wood boiler aerosol emissions, commercial aircraft jet engine PM emission profiles and PM profiles from the Kansas City Light-Duty Vehicle Emissions Study[6, 7]. SPECIATE emission profiles underpin the newest data set used by OAQPS to run its emission inventory and other models (i.e., the 2011 NEI modeling platform).

The need to support two important OTAQ efforts drove the need for the release of SPECIATE 4.4 in early 2014. These were the Tier 3 Vehicle Emission and Fuel Standards Program for the 2017 model year and the release of MOVES 2014. Even though speciation data are available in the associated dockets, they could be difficult to find. Release of these profiles in SPECIATE 4.4 made them more readily accessible and increased the transparency of the rulemaking process.

Additional significant uses of SPECIATE include:
- OAQPS recently developed composite source profiles for the pulp and paper industry using SPECIATE 4.4 profiles rather than a default speciation profile based on all of the emission sources contained in SPECIATE 3.2. The default profile is not a good fit for many source categories. The 2011 NEI Platform has over 150,000 tons of volatile organic

gases that are speciated using the default profile, providing a great opportunity to improve the inventory.

- Support of the Ozone NAAQS and the Transport Rule
- Support of updated rulemaking sensitivity analysis on impact of air quality modeling through use of SPECIATE profiles for emissions from ethanol fuels
- OTAQ's Tier 3 rulemaking and the National-Scale Air Toxics Assessment (NATA)
- Input to OTAQ's anti-backsliding study that needs newer profiles for upcoming ethanol fuel emissions analyses
- Providing a major reference in Tami Bond's 2004 black carbon emissions inventory paper and subsequently the Black Carbon Report to Congress[8, 9]
- A 2013 CMAS presentation of an analysis of the impact of ozone reactivity on air pollutant emission inventories[10].

Future Plans/SPECIATE 4.5

SPECIATE 4.5 will add more emission profiles and additional fields in the database as needs dictate. These profiles will capture recent and scientifically meritorious speciation profile data for VOC, TOG, PM and Other Gases that are available from EPA, state agencies, peer-reviewed literature, and other relevant data sources. As of March 2015, 54 speciated PM emission profiles have been added to SPECIATE 4.4 in anticipation of SPECIATE 4.5. These profiles included emissions from cook stoves, garbage burning, brick kilns, wood stoves, fireplaces, prescribed burning, coal combustion and welding fumes. For TOG, nine profiles have been added for oil and gas production, prescribed burning, petroleum refining, dairy operations and poultry production. At least 91 new chemical species have been added to the Species Properties table. These species were added for several emission sources including woodstoves and fireplaces.

Five potential data sources for TOG emission profiles have been identified for heavy-duty vehicles burning diesel and biodiesel fuels, new light-duty vehicles burning ethanol, and oil and gas production. Two potential data sources for PM have been identified for power plants and wood burning. The wood burning data set, along with two others already added to SPECIATE, include all of the dominant wood types burned in the entire United States. An extensive set of biomass combustion emissions speciation data was identified and requested from its developers. Task partners have also indicated the need for improved wildfire speciation factors.

Modification of the structure of the SPECIATE database will be considered to allow for storage of the additional important information underlying each profile (i.e. meta-data such as sampling and analysis methods and overall subjective profile quality ratings). The assignment of species to photochemical reactivity classes is being considered.

The Workgroup recognizes the need to develop new sector-based composite source profiles to associate more appropriate default speciation profiles to each SCC. Presently, many sources are matched to a default speciation profile based on an average source based on the all sources in SPECIATE 3.2. This significantly impacts results when processing emissions data with SMOKE and other emissions models.

A need for additional data on currently unspeciated organic emissions from combustion sources is being considered given their potential influence on inventories of secondary organic aerosols (SOA). Source sectors such as biomass burning, wood burning, on-road vehicles and off-road vehicles could contribute greatly to primary organic aerosol emissions and subsequent SOA production[11].

SPECIATE could support assessments of compounds important to global climate [e.g., methane (CH_4) and BC]. SPECIATE has been noted multiple times by our project partners as necessary for their emission inventory and modeling activities including plans to add elemental carbon (EC) and organic carbon (OC) to future national NEIs. BC and EC are aerosol classifications that are often used interchangeably. However, in practice the definition for BC may encompass organic carbon compounds that absorb light but are not purely graphitic. More analysis is needed to determine if current EC speciation profiles are appropriate for estimating BC emissions. If SPECIATE is to be used for CH_4 and BC emission estimates in the future, it will be critical to evaluate the profiles with radiative forcing metrics specifically in mind. Since CH_4 is not classified as a VOC by the EPA, previous evaluations of TOG speciation may not have focused particular attention on this compound. If CH_4 is considered to be a criteria air pollutant subject to the NAAQS in the future, SPECIATE will need to capture these emissions data[12].

SUMMARY

In February 2014, EPA released SPECIATE version 4.4. The primary purpose of each version of the SPECIATE database is 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. Each database revision stores important information underlying each profile (metadata such as sampling and analysis methods, overall subjective profile quality ratings, etc.). SPECIATE and its Web Browser capture and provide critical data needed to characterize emissions by species and source category. (See http://cfpub.epa.gov/si/speciate/[2].) The SPECIATE Web Browser makes it easy for users, who are not experienced in using MS Access, to view and use SPECIATE data. The SPECIATE 4.4 database can be downloaded from the EPA website at http://www.epa.gov/ttn/chief/software/speciate/index.html[5].

ACKNOWLEDGEMENTS

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KEYWORDS

SPECIATE, speciated emissions data, database, web browser, air pollution, A&WMA