

What's New in SPECIATE 4.2?

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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 source 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 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). This paper addresses Version 4.2 of the SPECIATE database that was completed in March 2008.

INTRODUCTION

The SPECIATE Database is an important EPA product which serves as the repository for source category-specific emission speciation profiles. The profiles contain weight fractions of species of both volatile organic compounds (VOC) and PM. The weight fractions of VOC species are grouped into reactivity classes to support air quality modeling for ozone. The profiles of PM species weight fractions are specific to particle size ranges and are being used to support air quality modeling for PM and visibility. The Database has also supported air toxic assessments and is essential for source-receptor modeling applications.

The Database was first computerized in 1988. Although accessibility to the Database has been sustained through the Clearing House for Inventories and Emission Factors (CHIEF) website, updates to SPECIATE have languished since the mid-1990s due to decreasing budgets. The U.S. National Research Council in its report on Research Priorities for Airborne Particulate Matter (2004)¹, the Clean Air Act Advisory Committee in its report of the Air Quality Management Working Group (December 2004)², the North American Research Strategy for Tropospheric Ozone in its Emission Inventory Assessment (September 2005)³, and other groups have recommended that the Database be extensively updated and maintained in a dynamic manner.

Given the importance of SPECIATE to the process of air quality management, a team was organized to undertake an update of the Database. The scope of the team's project was to: 1) update the Database with profiles from the literature and EPA source test data sets; 2) link the new profiles to Source Classification Codes (SCCs) in the National Emissions Inventory (NEI);

3) assign any new species to reactivity classes; and 4) update the air quality models to use the new information. SPECIATE version 4.0 was published in December 2006.

SPECIATE VERSION 4.2

The final report, “SPECIATE 4.2—Speciation Database Development Documentation (EPA/600-R-09/038, June 2009)”⁴ summarizes the development and provides guidance on use of the Database. The Database and final report are posted on the CHIEF Website, (<http://www.epa.gov/ttn/chief/software/speciate/index.html>).

This report documents how EPA developed the SPECIATE 4.2 database that updates the prior version of the SPECIATE 4.0 database. (There was an interim database, SPECIATE 4.1, which incorporated data from Environment Canada to the SPECIATE 4.0 database.) In total, there were 408 VOC profiles and 462 PM profiles appended to produce the SPECIATE 4.2 database. There was a change to the structure of the SPECIATE 4.2 database with the addition of the new category called Other Gases. This category contains speciated mercury, nitrogen oxides, and semivolatile organic compounds (SVOC) which do not fall into VOC and PM profiles categories. There were 237 Other Gases profiles incorporated into this version of the database. In addition, the report documents revisions to auxiliary data tables including the VOC-to-total organic gas (TOG) conversion table and the SCC-to-SPECIATE profile cross-reference table. The SPECIATE 4.2 database also contains a new table titled “SVOC Splitting Factors” which provides suggested SVOC partitioning factors in PM and gaseous phases based on a Schauer et al. study⁵. Note that the partitioning factor of each SVOC species is not universal. It depends on sampling conditions (e.g., temperature and pressure).

The primary purpose of this project was to update the SPECIATE databases 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. Another objective of this project was to modify the structure of the SPECIATE 3.2 database. The revised SPECIATE databases (i.e., versions 4.0, 4.1 and 4.2) allow for storage of important information underlying each profile (meta data such as sampling and analysis methods, overall subjective profile quality ratings, etc.). In addition, auxiliary data tables were also updated. These include the VOC-to-TOG conversion table and the SCC-to-SPECIATE profile cross-reference table.

The SPECIATE database and Work Group are contributing significantly to prioritizing activities of the emission inventory, air quality modeling, and emission testing programs. Much of this analysis emerged from the paper which is published in *Environmental Science and Technology*, "Emissions Inventory of PM_{2.5} Trace Elements across the United States," by Adam Reff, Prakash Bhawe, Heather Simon, Thompson Pace, George Pouliot, David Mobley, and Marc Houyoux (Publication Date: July 6, 2009, <http://pubs.acs.org/doi/abs/10.1021/es802930x>). As part of this analysis, some source categories identified as needing profiles, which are prioritized on our current list for inclusion in the next version (4.3) of database in the next Work Assignment which was initiated on July 1, 2009.

To date, the initiative to update SPECIATE has produced:

- 3,326 PM profiles (SPECIATE 4.2 database);
- 1,624 organic gas profiles (SPECIATE 4.2 database);
- 237 Other Gases profiles (SPECIATE 4.2 database);
- A total of 2,207 unique species (SPECIATE 4.2 database);
- Composite profiles for 58 (47 PM and 11 VOC) source categories (SPECIATE 4.2 database);
- An updated SCC-to-SPECIATE profile cross-reference table accounting for over 80 percent of national VOC and PM emissions in the 2002 NEI;
- VOC-to-TOG conversion factors for applicable gas profiles;
- A protocol for expansion of the database;
- Suggested partitioning factors for SVOC compounds in gas and PM phases;
- A mapping of the new VOC compounds into model species categories; and
- Review and prioritization of 49 studies entailing 614 PM and 822 VOC profiles for potential inclusion in the future SPECIATE database. The numbers do not include several large databases which need further investigation (e.g., California Air Resources Board light-duty gasoline exhaust annual surveillance tests which contain many hundreds of TOG profiles).

Progress of SPECIATE Database

	PM Profiles	Organic Gas Profiles	Other Gases Profiles	Numbers of Species	Released Year
Version 3.2	1,504	567	0	890	2002
Version 4.0	2,864	1,216	0	1,902	2007
Version 4.2	3,326	1,624	237	2,222	2009

SPECIATE DATA BROWSER

During 2008, a web-based application was developed in ColdFusion and Oracle to allow access to the SPECIATE database through a simple web interface. This web-based application can be accessed through the World Wide Web and facilitates direct download of SPECIATE source profiles (i.e., MS Access is not needed). The application allows data searches by pollutant, key word, and category. The SPECIATE Web Browser can be viewed here: <http://cfpub.epa.gov/si/speciate/>.

SUMMARY

SPECIATE 4.2 and its Data browser represent a significant enhancement of the data available to characterize emissions by species and source category. Air quality modeling and source-receptor modeling applications have benefited from using these enhanced speciation profiles. Additional efforts are needed to capture new data from current testing based on data submitted via the protocol for database expansion. The user community can support the Database development by supplying electronic data with full references.

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. The SPECIATE project is a work-in-progress; comments based on review of the database and documentation are welcome. Comments and questions may be directed to the EPA Manager, Mr. Lee Beck (Beck.Lee@epamail.epa.gov).

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