SPECIATE - EPA's Database of Speciated Emission Profiles

J. David Mobley, Lee L. Beck, Golam Sarwar, Adam Reff, and Marc Houyoux
U.S. Environmental Protection Agency, Research Triangle Park, NC

Abstract
SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of total organic compound (TOC) and particulate matter (PM) speciation profiles for emissions from air pollution sources. The profiles are key inputs to air quality modeling and source-receptor modeling applications. This paper addresses Version 4.0 of the SPECIATE Database.

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 Particulate Matter (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 US National Research Council in its report on Research Priorities for Airborne Particulate Matter (2004), the Clean Air Act Advisory Committee in its report of the Air Quality Management Working Group (December 2004), NARSTO in its Emission Inventory Assessment (September 2005), 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
The final report, "SPECIATE 4.0—Speciation Database Development Documentation (EPA/600/R-06/161, November 2006)" summarizes the development and provides guidance on use of the Database. The Database is posted on the CHIEF Website, (http://www.epa.gov/ttn/chief/software/speciate/index.html). The final version of the Database has been integrated into the Emissions Modeling Platform for subsequent research and regulatory modeling applications. The ability to speciate the emissions inventory with the new SPECIATE composite profiles will bring substantial benefits to the fields of air quality modeling and source apportionment, including:

- Support the creation of speciated emissions inventories for air quality modeling applications for fine particulate matter ($PM_{2.5}$), ozone (O_3), and regional haze;
- Estimate hazardous and toxic air pollutant emissions from total PM and VOC primary emissions;
- Support source-receptor modeling with chemical-mass balance models, positive matrix factorization, and factor analysis models;
- Verify profiles derived from receptor modeling using ambient measurements
- Facilitate source apportionment using air quality models by using source tagging of the trace elements and indicator species.

Results from these improved analyses will enable the development of more effective control strategies for sources of these species. Further, estimates of uncertainty in the results of air quality and receptor models will be improved by providing the most representative and up-to-date information to characterize emissions from the myriad point, area, mobile, and biogenic sources that contribute to ambient pollutant concentrations.

The initiative to update SPECIATE has produced:

- 2,856 PM profiles (1,503 legacy profiles, plus 1,258 new profiles including 95 simplified profiles);
- 1,215 gas profiles, 648 of which are new profiles;
- 1902 unique species, 1012 of which are new species;
- 58 Composite profiles for source categories (47 PM and 11 VOC);
- An updated cross-reference table linking profiles to source classification codes;
- VOC-to-TOG conversion factors for applicable gas profiles;
- A protocol for expansion of the Database;
- 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 future inclusion in the SPECIATE Database.

APPLICATIONS

The SPECIATE 4.0 Database has been integrated into the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, and its impact on predictions of ambient O_3 and PM concentrations has been evaluated by using the Community Multiscale Air Quality (CMAQ) modeling system. The results indicate that the new species profiles change the levels of predictions but do not change the levels significantly such that previous regulatory applications will be adversely impacted. In addition, the Database has been used to speciate $PM_{2.5}$ emissions for investigations into source-receptor modeling evaluations. The latter application of the improved database resulted in a national inventory of $PM_{2.5}$ emissions that is more resolved at both the chemical and source-category levels than any known before.

SUMMARY

SPECIATE 4.0 represents 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.

ACKNOWLEDGEMENTS

REFERENCES

NRC. 2004. Research Priorities for Airborne Particulate Matter: IV. Continuing Research Progress, National Research Council, National Academies Press, Washington, DC.

CAAAC. 2004. Recommendations to the Clean Air Act Advisory Committee, Air Quality Management Working Group, December 2005.

NARSTO. 2005. Improving Emission Inventories for Effective Air Quality Management Across North America—A NARSTO Assessment. NARSTO-05-001, September 2005.

US EPA. 2006. SPECIATE 4.0—Speciation Database Development Documentation. EPA/600/R-06/161, (http://www.epa.gov/ttn/chief/software/speciate/index.html), US Environmental Protection Agency, Research Triangle Park, NC, November 2006.