Objectives of the Research Project

The objectives of this research project were to review the applicability of the Chemical Mass Balance (CMB) receptor modeling and available source composition profiles for estimating source contributions to ambient VOCs using data from the Photochemical Assessment Monitoring Station (PAMS) networks and to develop a protocol for validation of ambient and source composition input data and for evaluation and interpretation of model outputs.

Summary of Findings

This document provides a protocol for applying the Chemical Mass Balance (CMB) receptor model to volatile organic compound (VOC) data from the Photochemical Assessment Monitoring Station (PAMS) networks and for evaluating and interpreting model outputs. The protocol provides recommended procedures for validating ambient VOC data, assigning uncertainties to ambient and source measurements, selecting and evaluating source composition profiles and fitting species, evaluating and validating model outputs, and analyzing and interpreting the CMB source contribution estimates and associated uncertainties. The CMB applications and validation protocol developed by Watson et al. (1998) was adapted here for application to PAMS and similar VOC data.

The guidance includes a current library of available source VOC composition profiles in CMB8-ready format and sample CMB Version 8 VOC source and ambient input data files. The profiles are contained in the file CMBProfilesLibrary.xls. This library is a compilation of source profiles that have been used by the Desert Research Institute in prior VOC source apportionment studies. They include profiles that were newly developed for specific studies, the literature, and from the California Air Resources Boards Modeling Emissions Data System (MEDS). Studies for which profiles were newly developed include the 1993 Coast Oxidant Assessment for Southeast Texas (Fujita et al., 1995b), 1995 Boston and Los Angeles VOC Source Apportionment Study (Fujita et al. 1997a), 1995/96 Washington Ozone Transport Study (Fujita et al., 1997c), 1996 El Paso/Juarez Ozone Study (Fujita, 2001; Seila et al., 2001), and 1998 Central Texas On-Road Hydrocarbon Study (1999a), 1999 VOC Source Signatures in Houston, (Fujita et al., 1999b), apportionment of 1994-97 South Coast Air Basin PAMS VOC data (Fujita and Campbell, 2003), and the 2000 Weekend Ozone Observations in the South Coast Air Basin (Fujita et al. 2002; Fujita et al., 2003a). The document and supporting files are intended to facilitate and encourage the application of the CMB receptor model to PAMS VOC data by State and Local air pollution agencies as an evaluation of emissions inventories.
The profiles are expressed as weight fractions and are normalized to the sum of the 55 PAMS target hydrocarbons. The PAMS species typically account about 80 percent of the total ambient hydrocarbons in urban locations, and their sum is more reproducible among different laboratories than total NMHC or NMOC. Compounds other than the 55 Photochemical Assessment Monitoring Station (PAMS) target NMHCs that are individually identified are grouped into a category named “other”. Compounds reported as “unknowns” are grouped into a category named "UNID". The profiles also include total NMHC (i.e., the sum of PAMS species + other + unid) normalized to sum of PAMS species. Although not measured in the PAMS program, methyl tert-butyl ether (MTBE) is included in the profiles because it is a major component in reformulated gasoline and in the exhaust of vehicles using RFG. By including MTBE in the profile, its ambient concentration can be predicted by CMB.

To assist with the selection of profiles, several sort fields are included such as category (source type), location and year. The list of profiles can be filtered by selecting values from any or all of these fields using the pull down menus on each heading. Up to four profiles can be compared graphically in a set of three column plots. Two of the plots contain the 55 PAMS species and all other organic species, respectively, for the selected profiles. A third plot shows a detailed comparison of the typical major species for the first two profiles selected. Running a macro in the source profile data file automatically generates the source profile, source selection and species selection files.

Procedures for evaluating the validity of the application of CMB to PAMS VOC data includes: 1) determination of model applicability; 2) review of initial source contribution estimates; 3) examination of model outputs and performance measures; 4) identification of deviations from model assumptions; 5) identification and correction of model input errors; 6) verification of the consistency and stability of source contribution estimates; and 7) evaluation of the results of the CMB analysis with respect to other source assessment methods.

Publications and Presentations

The results of several studies were used in the development of the application and validation protocol for VOC source apportionment and compilation of the VOC source composition library. The following is a list of relevant journal publications, reports and presentations. While some of the projects predate this study, most overlap this study in time and influenced the development of the protocol.

Publications


Reports


Watson, J.G., Robinson, N.F., Lewis, C.W., Coulter, C.T., Chow, J.C., Fujita, E.M., Conner, T.L., Pace, T.G. (1998a). CMB8 applications and validation protocol for PM$_{2.5}$ and VOCs. Report No. 1808.2D1, Desert Research Institute, Reno, NV.


Presentations


**Supplemental Keywords**

Chemical Mass Balance  
receptor model  
source apportionment  
source attribution  
source composition profiles  
volatile organic compounds (VOC)  
Photochemical Assessment Monitoring Stations (PAMS)

**Relevant Web Sites**

This document, the CMBProfilesLibrary file and a self-extracting zipfile (SoCAB.exe) containing sample CMB input files with ambient and source VOC datasets for California’s South Coast Air Basin are available at the Desert Research Institute web site at [http://www.dri.edu/People/ericf/](http://www.dri.edu/People/ericf/). Specific questions and comments regarding this document and sample datasets may be addressed to Dr. Eric Fujita at [ericf@dri.edu](mailto:ericf@dri.edu). The CMB software is available at the TTN web site at [http://www.epa.gov/scram001/tt23.htm](http://www.epa.gov/scram001/tt23.htm). Questions regarding the CMB software should be directed to Dr. John Watson at DRI at [johnw@dri.edu](mailto:johnw@dri.edu).