

**PEER REVIEW OF THE  
CHEMICAL MASS BALANCE MODEL (EPA-CMB8.2)  
AND DOCUMENTATION**

**U.S. ENVIRONMENTAL PROTECTION AGENCY**

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*Under EPA Requisition No. U2C761*

## PREFACE

The U.S. Environmental Protection Agency, through their contractor, commissioned a panel of three reviewers to assess the documentation, performance and user friendliness of the Chemical Mass Balance Model, (EPA-CMB8.2). EPA is interested in recommending the adoption of EPA-CMB8.2 as a replacement for CMB7 for regulatory applications during the implementation EPA's particulate matter (PM) programs. A panel of three reviewers, Mr. James J. Schauer, Ph.D., Ms. Donna M. Kenski, Ph.D., and Mr. Robert D. Willis, Ph.D. were retained as outside contractors to provide independent review.

This report responds to EPA's "Charge to Reviewers" by providing summarized primary conclusions and comments resulting from the peer review. Included with the report as appendices are supporting information including a copy of the EPA "Charge to Reviewers" (Appendix A), an overview of the peer review process (Appendix B), qualifications and background information on the review panel members (Appendix C) and a copy of each reviewers specific comments (Appendix D).

The materials reviewed included the draft reports entitled;

- *EPA-CMB8.2 User's Manual*, September, 2004
- *Protocol for Applying and Validating EPA-CMB8.21 to PM-2.5 and VOC*
- An electronic copy of EPA-CMB8.2 installation utility, and all the model source code
- Electronic copies of properly formatted test data sets, including; Boston, Houston, Portland Aerosol Characterization Study (PACS)<sup>1</sup>, Northern Front Range Air Quality Study (NFRAQS), and Jan Joaquin Valley Fine (SJVF)<sup>2</sup>

These documents and software were provided by Tom Coulter, HEASD/Environmental Characterization & Apportionment Branch (E205-03), National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC.

The KEVRIC Company Inc. provided the administrative management necessary to conduct this peer review. KEVRIC's efforts are outlined in the overview of the process included as Appendix B.

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1 The FINE/COARSE/TOTAL functionality described in Section 3.6.1 and 4.2.3 of the *EPA-CMB8.2 User's Manual* is based on this data set.

2 The test case described in Section 5 of the *EPA-CMB8.2 User's Manual* is based on this data set. Demonstration of the multiple size range treatment described in Section 4.2.3 is based on data synthesized from this data set.

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## 1.0 INTRODUCTION

The Chemical Mass Balance (CMB) air quality model is one of several receptor models that have been applied to air resources management. Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations. Receptor models are generally contrasted with dispersion models that use pollutant emissions rate estimates, meteorological transport, and chemical transformation mechanism to estimate the contribution of each source to receptor concentrations. The two types of models are complementary, with each type having strengths that compensate for the weaknesses of the other.

The CMB receptor model was first applied by Winchester and Nifong (1971), Hidy and Friedlander (1972), and Kneip *et al.* (1973). The original applications used unique chemical species associated with each source-type, the so-called “tracer” solution. Friedlander (1973) introduced the ordinary weighted least-squares solution to the CMB equations, and this had the advantages of relaxing the constraint of a unique species in each source-type and of providing estimates of uncertainties associated with the source contributions. The ordinary weighted least squares solution was limited in that only the uncertainties of the receptor concentrations were considered; the uncertainties of the source profiles, which were typically much higher than the uncertainties of the receptor concentrations, were neglected.

The first interactive, user-oriented software for CMB was programmed in 1978 at the Oregon Graduate Center in FORTRAN IV on a PRIME 300 minicomputer (Watson, 1979). The PRIME 300 was limited to 3 megabytes of storage and 64 kilobytes of random access memory. CMB Versions 1 through 6 updated this original version and were subject to many of the limitations dictated by the original computing system. CMB 7 was completely rewritten in a combination of the C and FORTRAN languages for DOS-based microcomputers with floating-point coprocessors, hard disk systems with tens of megabytes of storage, and available memory of 640 kilobytes. CMB8 was developed but not officially released by EPA. CMB8 created a user interface for CMB7 calculations using the Borland Delphi object oriented language.

EPA-CMB8.2 incorporates the upgrade features the CMB8 has over CMB7, but also corrects error/problems identified with CMB8 and adds enhancements for a more robust and user-friendly system.

The purpose of this document is to assist EPA by providing a scientific peer review to assess the modeling system's documentation, performance, and user friendliness. This review is ambitious given time and resource limitations. Unlike a traditional scientific peer review (e.g., for a refereed journal) this review does not attempt to verify or challenge each statement, equation, or data set in the report-- rather, it is a careful consideration of the overall user-friendliness and accuracy, usefulness of documentation in light of the use of the modeling system by users for regulatory applications. EPA, through its contractor, provided guidance to the reviewers in its "Charge to Peer Reviewers", which is attached to this report as Appendix A.

Following this introduction, Section 2, entitled "Summary of Peer Review Comments," summarizes the reviewers' responses to the "Charge to Peer Reviewers". Each reviewer's individual comments on the Reports are found in Appendix D. Unless otherwise noted, this report represents a consensus of all three reviewers.

## 2.0 SUMMARY OF PEER REVIEW COMMENTS

This section presents a summary consolidation of the primary peer reviewer's comments on EPA-CMB8.2. This summary review focuses on the major points raised by the three reviewers and is not a comprehensive summary of all comments. The individual reviews are included as Appendix D of this report. The peer review of the EPA-CMB8.2 software consisted of review of the following materials provided to the peer reviewers by EPA;

- *EPA-CMB8.2 User's Manual*, September, 2004
- *Protocol for Applying and Validating EPA-CMB8.23 to PM-2.5 and VOC*
- An electronic copy of EPA-CMB8.2 installation utility, and all the model source code
- Electronic copies of properly formatted test data sets, including; Boston, Houston, Portland Aerosol Characterization Study (PACS)<sup>3</sup>, Northern Front Range Air Quality Study (NFRAQS), and Jan Joaquin Valley Fine (SJVF)<sup>4</sup>

The review also included running the EPA-CMB8.2 software with datasets provided by EPA as well as datasets and run files created by the reviewers.

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<sup>3</sup> The FINE/COARSE/TOTAL functionality described in Section 3.6.1 and 4.2.3 of the *EPA-CMB8.2 User's Manual* is based on this data set.

<sup>4</sup> The test case described in Section 5 of the *EPA-CMB8.2 User's Manual* is based on this data set. Demonstration of the multiple size range treatment described in Section 4.2.3 is based on data synthesized from this data set.

All three reviews agreed that the EPA-CMB8.2 is a significant improvement over previous version of EPA's CMB software releases. EPA-CMB8.2 effectively takes advantage of the Windows® operating systems, which allows users to efficiently create input files, efficiently operate the model, and efficiently review and analyze the model results within the framework of the software and through software output files. Relative to other air quality modeling software and other specialized technical software, EPA-CMB8.2 is very user friendly and flexible to meet the broad needs of the air quality field. The manuals provide a solid foundation on the appropriate use of the EPA-CMB8.2 and the theoretical and statistical basis for the model, as well as excellent reference lists for CMB users who need additional information. The CMB input files provided with the model provide an excellent training tool for new users and provide an ideal reference for users that are developing new input files.

The peer reviewer's identified several issues with regard to the EPA-CMB8.2 software and manuals of which they deem represent critical problems with the EPA-CMB8.2 software and manuals. It is their opinion that these issues present potential for misuse of the system which might yield erroneous results, and therefore, they recommend these issues be resolved prior to release of the software. Several other issues were identified which, in the opinion of the peer reviewers, represent inconveniences with the software and manuals that make the software less user friendly, and should be corrected, if possible, but are not obstacles to the release of EPA-CMB8.2. The peer reviewers also identified issues that were deemed to be problems with EPA-CMB8.2 that existed with previous versions of the software, (i.e., carry-over issues) that were not addressed in the upgrade. The peer review team presents these carry-over issues in order to make EPA aware, however, it is the opinion of the peer review team that these issues are not considered obstacles to the release of EPA-CMB8.2. The following sections present the critical, software inconvenience and carry-over issues and supporting information.

## **2.1 Critical Issues**

2.1.1 The operation of the EPA-CMB8.2 model without a run file (i.e. the manual selection of input files) has some major flaws that make the model inoperable in this mode. The EPA-CMB8.2 software and associated manual explicitly state that the user should use this mode with caution. Nonetheless, the problems with this operating mode are significant and should be removed or the user should be told what problems to expect. The most significant problem observed with this mode is the shifting and/or misalignment with labels during interactive use of the source profile and species selection windows. This problem has also been identified to occur while using a control file (see 2.1.2 below). This problem

effectively makes the model inoperable without significant sidestepping of software operations. Specific information on how the files were run for this problem to occur is provided within Jamie Schauer's individual comments, included in Appendix D of this report.

2.1.2 If a species or source array is modified within CMB and then highlighted, the modified array (or any other array) or run a fit, the changed species or source is moved to the bottom of the arrays. For example, modify species array #1. Now perform a fit with the modified array. The species used in the fit are the same as those selected in array 1, but if you examine array1, the changed species is now at the bottom of the array. Now click on array 1. Nothing changes visibly with array 1, but if you repeat the fit, the fitting species have changed! And if you select any other species array and perform a fit, the actual fitting species are different from what the array shows as being selected. And if you save the selection file after performing a fit, the saved file does not work properly.

2.1.3 No control file was provided for the NARSTO and COAST test data and there seems to be some errors with these files as the provided files will not run properly.

2.1.4 More explanation of the Britt-Luecke algorithm testing needs to be presented on page 3-5 and X-Y of the *EPA-CMB8.2 User's Manual*. It is unclear if the insufficient testing is for the EPA-CMB8.2 software code or the application to CMB calculations. Although the manual provides adequate precautions, the manual should provide more information to insure that the user understands the precautions more completely.

2.1.4 Section 6.1.2, pages 6-4 through 6-5 of the *EPA-CMB8.2 User's Manual*: More discussion on the appropriate setting for maximum source uncertainty and minimum source projection is needed. In several places in the manual, it is stated that hard-wired CMB7 values were appropriate for PM that used XRF data, but that these values are not appropriate for VOC data and presumable other analytical methods. As a minimum, some recommendations should be offered for VOC data. In addition, the implication of changing these values needs to be presented.

2.1.6 Appendix G of the *EPA-CMB8.2 User's Manual*: The information about the EST parameter needs to be moved to the main body of the manual. The implication of the "lack of understanding of the EST parameter" on selection of source elimination needs to be discussed as well.

2.1.7 Calculated fit measures do not agree with the formula on page 6-10 of the *EPA-CMB8.2 User's Manual*. You can see what the program is doing by successively zeroing all weights but one and re-running a fit. The Fit Measure (FM) is correct when Rsq and %Mass are the only weighted parameters. The FM is a factor of 2 in error when  $\chi^2$  is the only weighted parameter, and FM goes bonkers when Fraction Estimate is the only weighted parameter.

2.1.8 The FM formula on page 6-10 of the *EPA-CMB8.2 User's Manual* appears to be wrong, aside from the question of what is the correct weighting for  $\chi^2$ . Shouldn't the entire expression be divided by a normalization factor equal to the sum of the weights?

2.1.9 The "source projections" do not appear to operate as described in the *EPA-CMB8.2 User's Manual*. The output appears to be inconsistent, at least at times, with the identification (YES or NO) that a source is estimable. An example includes a base case model run (i.e. default sources and species) using the NFRAQS Bright sample from 12/15/96 that started at 0600. Source N010 is identified as non-estimable, yet its source projection is listed as 0.9987, greater than the 0.95 threshold for an estimable source.

2.1.10 CSV and TXT output files are not identical in the last two columns, and both are missing data. Example: run CMB with INsjvf.in8 control file. Run. File, Save current record only as \*.txt file. Now, go to Options and select \*.csv output format. Run. File, Save current record only as \*.csv file. Compare .txt and .csv files in Excel. They differ in the last two columns. The csv file has column headings but no data for SJV065 and Soil 31. The txt file has neither data nor column headings for this source. This source was unselected in the selection file. However, selecting this source and re-running the results as before makes no difference: both output files are missing data for this last source.

## 2.2 Software Inconveniences

2.2.1 The one major drawback with the EPA-CMB8.2 software is the unforgiving process of building a set of input files that software will accept. Once the files are acceptable to the program, running them seems to go smoothly and without major glitches; the few error messages that cropped up were simple to deal with. Although the EPA-CMB8.2 software has a series of checks that provide well described and documented error messages, many formatting problems with the input files are not identified by the EPA-CMB8.2 software and these problems ultimately lead to software errors that provide cryptic descriptions, resulting in frustration for the user. Although it seems impractical for EPA to revise EPA-CMB8.2 to



catch all of these potential errors, EPA should consider the possibility of developing a simple formatting-check software that could read in all of the CMB 8.2 input files and check formatting and data framework consistencies. This would make a huge contribution toward trouble shooting of EPA-CMB8.2.

2.2.2 EPA should be commended for provided five complete sets of EPA-CMB8.2 input files for the user to test and review. If EPA intends to include these data sets with the software release then EPA needs to properly warn users that the data sets and their associated results presented in the manual have not been peer reviewed.

2.2.3 Some error messages are cryptic and not very helpful. Example: “Column (source) Number [] of Afit = 0.” Could you instead say “Source xxx has zero concentrations for all species. Change the source profile or remove the source”? Another example: “AKT\*VeffIn\*AK matrix needs improvement...”. Can you say instead: “Two or more sources are probably collinear. Change fitting sources or fitting species to remove the collinearity”? Also, if some error messages are potentially misleading, can’t they be changed to be more helpful?

2.2.4 Data box which accompanies the graphs of sources or samples won’t display all species if you have a large number of species. It seems that a scroll button is needed.

2.2.5 Missing data (-99.) in source profiles or ambient data show up numerically as -99 in View Graph plots. This effectively renders the graph useless for the other species.

2.2.6 The graphical output that was part of the original CMB8, including time-series bar charts and source contribution pie charts, are greatly missed in the present version. Also, “Present Computed Averages” is gone. These were useful features and would be a significant enhancement to the 8.2 version.

2.2.7 CMB7.0 quantitatively estimated the source contributions of sources that were found to be co-linear with the model using similarity clusters. This option has been dropped in the CMB8 versions and there is currently no quantitative method for dealing with co-linear source profiles in the model. EPA should consider adding back in the feature or provide the user a quantitative method to deal with co-linear source profiles.

## 2.3 Carry-Over Issues

2.3.1 More discussion on the appropriate use of source elimination is needed on page 3-5 and page 6-2 of the *EPA-CMB8.2 User's Manual*. The user should be warned that they should not just use source elimination as a starting point. Proper CMB analysis requires an understanding of why sources are being removed. The removal of a source for colinearity purposes is not the same as removal due to negative but not statistically significant source contributions. In addition, removal of sources without removal of tracers can often lead to violation of source completeness for specific tracers.

2.3.2 Section 6.1.1, pages 6-2 through 6-3 of the *EPA-CMB8.2 User's Manual*. The basis for the acceptable criteria for R-square and chi-square needs to be provided. In addition, the C/M ratios should be added as performance criteria. In addition, the statement that percent mass should be in the range of 80% to 120% is not a fair criteria. A model can be very accurate, even exact, if some sources are missing from the model AND the missing sources are not contributors to the fitting species. A perfect example is the absence of secondary inorganic species from a CMB model.

2.3.3 Sec. 4.2.3 of the *EPA-CMB8.2 User's Manual*: The names of the variables are apparently more restricted than the manual indicates here, in length and characters allowed. The manual needs to be more specific about exactly what variable names are supported.

2.3.4 The meanings of column headings for the output file are not immediately obvious. An example, with descriptions, should be added to the manual, perhaps in Section 5 or alternatively, in Section 4.3.2 of the *EPA-CMB8.2 User's Manual*. At least add a note in Section 5 explaining that the output file is described in detail in 4.3.2 of the *EPA-CMB8.2 User's Manual*.

## 3.0 SUMMARY/CONCLUSIONS

In summary, all members of the peer review team reviews agreed that the EPA-CMB8.2 is a significant improvement over previous version of EPA's CMB software releases, and that relative to other air quality modeling software and other specialized technical software, EPA-CMB8.2 is very user friendly and flexible to meet the broad needs of the air quality field. The documentation provides a solid foundation on the appropriate use of the EPA-CMB8.2 and the theoretical and statistical basis for the model, as well as excellent reference lists for CMB users who need additional information.

*Peer Review of EPA-CMB8.2*

This peer reviewer identified several issues with regard to the EPA-CMB8.2 software and manuals of which they deem represent critical problems with the EPA-CMB8.2 software and manuals. It is their opinion that these issues present potential for misuse of the system which might yield erroneous results, and therefore, they recommend these issues be resolved prior to release of the software. Several other issues were identified which were considered by the peer reviewers to be inconveniences with the software and manuals, or carry-over problems from previous CMB model versions. The peer reviewers indicated that these issues should be corrected, if possible, but are not obstacles to the release of EPA-CMB8.2.

**APPENDIX A**

**EPA'S CHARGE TO REVIEWERS**

## Charge to Peer Reviewers

EPA is recommending the use of EPA-CMB8.2 for regulatory applications and this model is crucial for implementation of its PM program. It is therefore prudent that a science peer review be done to assess the modeling system's documentation, existing performance evaluations, and user friendliness. As a reviewer, you will install EPA-CMB8.2 according to the guidance in Section 2 of the *EPA-CMB8.2 User's Manual*.

### 1. Documentation

- a. Is the content and organization of the *EPA-CMB8.2 User's Manual* adequate? Are the model formulations, programming notes, and catalogue of warning/error messages sufficiently documented for technical critique and understanding?
- b. Is the discussion and presentation of the model and its features clear? Please note any specific sections of the documentation that were unclear or confusing.
- c. Is the documentation sufficient to guide a typical user in the use of the model?
- d. Is the content and organization of the *Protocol for Applying and Validating EPA-CMB8.2 to PM-2.5 and VOC* adequate? Does the protocol mesh well with EPA-CMB8.2 and user's manual (e.g., consistent terminology)? Are the appendices, i.e., 54 PAMS target compounds (hydrocarbons) listed in their elution sequence, Normalization for the VOC Source Profile, Internet Links to Modeling Software and Data Sets, Summary of CMB PM<sub>10</sub> Source Apportionment Studies, Summary of CMB VOC Source Apportionment Studies and Procedures for Treating Secondary Particles helpful? Are any in need of revision or enhancement? If so, how specifically?

### 2. Performance Evaluation<sup>5</sup>

Using the SJVF data set provided, the reviewer will perform the test case described in Section 5 of the *EPA-CMB8.2 User's Manual*. Does the test case tutorial behave as the manual describes?

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<sup>5</sup>The extent to which the CMB model has been evaluated with independent data sets is relatively unknown, and availability of suitable data is limited. EPA is unaware of any evaluation that has assessed CMB's treatment of secondary pollutants or aged aerosols, or of systematic perturbation of CMB's input data (e.g., randomized alteration of uncertainty values). EPA welcomes any specific recommendation regarding the kind of validation study that could/should be performed, using perhaps a synthetic data set.

Are there any surprises or anomalies? If so, please document accurately so that the Agency representative can reproduce the problem.

- a. Using the other data sets provided, the reviewer will load applicable Control Files and test behavior and performance against guidance presented in the *EPA-CMB8.2 User's Manual*. Results will be saved and examined using the appropriate viewing/editing software. Before closing a session (exiting), the reviewer will, on the **Select Input Files** screen, choose the respective Control File for the next data set. Is the behavior consistent with the guidance and information presented in the manual? When the Main Report is printed, does the output look normal or were there any other problems? When it is exported (printed to file) and examined, is the information consistent with that presented on-screen. Are there any surprises or anomalies? If so, please document accurately so that the Agency representative can reproduce the problem.
- b. Using one data set of his/her own propriety, the reviewer will test a properly formatted data set for the same conditions specified in (b) above. Was there aberrant behavior? Was there any trouble in EPA-CMB8.2's attempt to load the Control File, or in accessing the input data? Were the computation results the same as those seen in another version of CMB, e.g., CMB8? Again, please accurately document (including furnishing input data) so that the Agency representative can reproduce the problem.
- c. Stability. During any given session, or in moving from one data set to another by selecting a different Control File in the **Select Input Files** screen, was there any evidence of instability? Was there any condition that resulted in the system locking up (persistent hourglass), requiring a complete reboot? Again, please accurately document so that the Agency representative can reproduce the problem.

### 3. User Friendliness of Entire System

In building EPA-CMB8.2, EPA has endeavored to create a User Interface that logically facilitates the set up and run of an apportionment calculation. The UI is also configured to speed the process of examining preliminary fitting results, changing input conditions and re-running in iterative fashion until fitting statistics are optimized. Nevertheless, it would be useful to know:

- a. Are there any additional "user friendliness" concerns that should be addressed before release?
- b. If 'yes' to (a.), what specifically needs to be addressed?

**APPENDIX B**

**OVERVIEW OF THE PEER REVIEW PROCESS**

**OVERVIEW OF THE PEER REVIEW PROCESS  
for the  
PEER REVIEW OF THE CHEMICAL MASS BALANCE MODEL (EPA-CMB8.2) AND  
DOCUMENTATION**

The US Environmental Protection Agency, HEASD/Environmental Characterization & Apportionment Branch, in an effort to provide for independent, credible peer reviews of air dispersion models and studies retained a contractor, The KEVRIC Company Inc. of Silver Spring MD/Durham, NC to manage and coordinate the peer review project.

The peer review as handled as a work assignment under a contract with the KEVRIC Company. Once the work assignment was issued, KEVRIC prepared a detailed work plan for the approval of the Work Assignment Manager (WAM). For the EPA\_CMB8.2 project the official WAM was Tom Coulter.

The work plan provided a description of the tasks to be completed, the estimated time frame and estimated manhours/cost requirements. The description below describes the process by which the peer review for the EPA-CMB8.2 model and documentation was conducted.

The information provided to KEVRIC under the Work Assignment Statement of Work included;

- a “Charge to Reviewers”, formulated by EPA, that outline the specific direction and technical scope of the task for the peer review team.
- a list of qualified candidates, as known to EPA
- a list of materials to provided to the peer reviewers by KEVRIC/EPA

KEVRIC contacted several persons on the qualified candidate list, described the project to them and requested their participation based on their interest and availability. Three candidates were retained, Mr. James J. (Jamie) Schauer, PhD., P.E., Ms. Donna M Kenski, Ph.D., and Mr. Robert Willis, Ph.D. Mr. Schauer consented to act as chairperson, in that he would, in addition to providing peer review, compile a report that would summarize all of the peer reviewers comments and opinions into one concise report. This peer review team was approved by the acting WAM.

KEVRIC provided a sub-contract mechanism for the peer reviewers to be compensated for their time. It was estimated that each peer reviewer would spend up to 32 hours on the review and Mr. Schauer would spend an additional 16 hours compiling a report.

KEVRIC then arranged for the review materials to be reproduced and distributed to each reviewer. The materials provided to be reviewed were those provided to KEVRIC by USEPA as provided under the work assignment. These materials were as follows:

- *EPA-CMB8.2 User’s Manual*, September, 2004
- *Protocol for Applying and Validating EPA-CMB8.2 to PM-2.5 and VOC*
- An electronic copy of EPA-CMB8.2 installation utility, and all the model source code
- Electronic copies of properly formatted test data sets, including; Boston, Houston, Portland Aerosol Characterization Study (PACS), Northern Front Range Air Quality Study (NFRAQS), and Jan Joaquin Valley Fine (SJVF)



Once these materials were distributed, KEVRIC scheduled a teleconference call which involved the team members, V. Hanzel of KEVRIC, and Tom Coulter of EPA. The conference call was conducted to discuss the charge to the reviewers and establish commonality in the peer reviewer's efforts and to initiate the peer review.

The peer reviewers were instructed to perform their review according to the "Charge to Reviewers". It was agreed that contact amongst them was permissible and encouraged and all correspondence would be documented by emails.

After the reviewers provided comment, a draft report was compiled by Mr. Schauer that provided a summary of the opinions of the team and specific individual comment, as appropriate. This report was distributed via email to all parties for their review.

A second conference call was scheduled by KEVRIC to discuss the draft report and determine if any changes, modifications or clarifications were needed. Mr. Schauer revised the draft report and redistributed the final version to the team members.

The final version of the report was compiled, reproduced and submitted to EPA by KEVRIC. This compilation included addition of other documentation such as resumes of the reviewers and this overview of the process.

**APPENDIX C**

**PEER REVIEW PANEL**

**QUALIFICATIONS AND BACKGROUND INFORMATION**

## BIOGRAPHICAL SKETCH

**James Jay Schauer, Ph.D., PE**

Associate Professor, Department of Civil and Environmental Engineering  
University of Wisconsin-Madison

Director, Air Chemistry, Wisconsin State Laboratory of Hygiene

Water Chemistry Laboratory  
660 N. Park St.  
Madison, WI 53706

Tel: (608) 262-4495  
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email: jschauer@enr.wisc.edu

### Education:

B.S., Chemical and Petroleum Refining Engineering, Colorado School of Mines, 1984

M.S., Environmental Engineering, University of California at Berkeley, 1991

Ph.D., Environmental Engineering Science, California Institute of Technology, 1998

### Professional Experience:

6/04-Present Associate Professor, University of Wisconsin-Madison, Madison, WI  
Civil and Environmental Engineering, Environmental Chemistry Program,  
and The Wisconsin State Laboratory of Hygiene

10/98-6/04 Assistant Professor, University of Wisconsin-Madison, Madison, WI

3/98-9/98 Postdoctoral Scholar, California Institute of Technology, Pasadena, CA  
Environmental Engineering Science

8/93-3/98 Research Assistant, California Institute of Technology, Pasadena, CA  
Environmental Engineering Science

5/92-8/93 Development Specialist, UOP, Des Plaines, IL  
*Job Function:* Development of process technology for petroleum refining,  
petrochemical processes and environmental control.

8/86-5/92 Technical Advisor/Chief Technical Advisor, UOP, Des Plaines, IL  
*Job Function:* Start-up and commissioning of UOP process units in petroleum  
refineries and petrochemical processing facilities in Europe, Asia, Africa, and  
North America.

3/85-8/86 Development Engineer, UOP, Des Plaines, IL

### Teaching

CEE320 Environmental Engineering (Fall, 3 Credits)

CEE423/ME466 Air Pollution: Effects, Measurement, and Control (Spring, 3 Credits)

CEE609 Chemistry of Air Pollution (Fall, 2 Credits)

CEE629 Air Pollution and Aerosols Laboratory (Fall, 2 Credits)

CEE909 Water Chemistry Seminar (Spring and Fall, 1 Credit)

### Technical Expertise:

Measurement of emissions from air pollution sources  
Measurement of atmospheric pollutants  
Semi-volatile organic compound sampling  
ICP/MS analysis of airborne trace metals  
GC/MS analysis of atmospheric samples and air pollution source emissions  
Use of organic compounds as molecular markers in the environment  
Chemical mass balance (CMB) modeling  
Chemistry of petroleum based fuels

## Curriculum vitae, James Jay Schauer, page 2

### Technical Consulting:

- 9/98-2/99 US EPA Emissions Characterization & Prevention Branch, APPCD, NRMRL. Technical support for the start up of a program to measure chemical and physical properties of air pollution emissions for source apportionment studies  
Project Officer: Dr. Norman Dean Smith
- 1/00-12/00 US DOE National Renewable Energy Laboratory (NREL) and the Coordinated Research Council (CRC). Technical Support for the design of a source apportionment study for motor vehicles.  
Project Officer: Dr. Doug Lawson
- 12/01-6/02 Engine Manufacturers Association (EMA). Technical report writing covering the use of elemental carbon as a tracer to diesel particulate matter.  
Project Officer: Joe Suchecki
- 08/04-12/04 US EPA Office of Air Quality and Planning and Standards. Technical report writing covering the use of molecular marker for source apportionment of carbonaceous aerosols  
Project Officer: JoAnn Rice
- 10/04-12/05 Technical University of Vienna. Technical support for organic aerosol analysis and fine particle source attribution modeling  
Project Officer: Prof. Hans Puxbaum

### Awards

- 2004 Guest Professor Peking University (also known as Beijing University), Beijing, China
- 2002 Health Effects Institute (HEI) Rosenblith Young Investigator Award
- 2001 Haagen-Smit Award presented by *Atmospheric Environment* Journal in recognition of 1996 publication for contribution to the field of atmospheric sciences.

### Professional Affiliation:

- Associate Editor, Journal of Environmental Engineering and Science, NRC Canada  
Editorial Advisory Board, Aerosol Science and Technology (AS&T)  
American Chemical Society (ACS)  
American Association for Aerosol Research (AAAR)  
American Geophysical Union (AGU)  
Air and Waste Management Association (A&WMA)

### Registered Professional Engineer

- Colorado PE License # 27717  
Illinois PE License # 062-051408

### Peer Reviewed Journal Publications

- 1) G. C. Lough, J. J. Schauer, J. S. Park, M. M. Shafer, J. T. DeMinter, and J. P. Weinstein, 2004. Emissions of Metals Associated with Motor Vehicle Roadways. *Environmental Science and Technology*, In Press.
- 2) R. J. Sheesley, J. J. Schauer, E. Bean, and D. Kenski. 2004. Trends in Secondary Organic Aerosol at a Remote Site in Michigan's Upper Peninsula. *Environmental Science and Technology*, In Press.

- 3) J. Xu, M. H. Bergin, J. L. Jaffrezo, G. Aymoz, J. Zhang, and J. J. Schauer, 2004. Aerosol Chemical and Radiative Characteristics Near A Desert Source Region During ACE-Asia. *Journal of Geophysical Research-Atmospheres*, 109, Art. No. D19S03.
- 4) A. P. Sullivan, R. J. Weber, A. L. Clements, J. R. Turner, M. S. Bae, J. J. Schauer. 2004. A method for on-line measurement of water-soluble organic carbon in ambient aerosol particles: Results from an urban site. *Geophysical Research Letters*, 31, Art. No. L13105.
- 5) J. D. McDonald, E. B. Barr, R. K. White, J. C. Chow, J. J. Schauer, B. Zlienska, E. Grosjean, 2004. Generation and Characterization of Four Dilutions of Diesel Engine Exhaust for a Subchronic Inhalation Study. *Environmental Science and Technology*, 38, 2513-2522.
- 6) M. S. Bae, J. J. Schauer, J. T. DeMinter, and J. R. Turner, 2004. Hourly and Daily Patterns of Particle-Phase Organic and Elemental Carbon Concentrations in the Urban Atmosphere. *Journal of the Air and Waste Management Association*, 54, 823-833.
- 7) M. S. Bae, J. J. Schauer, J. T. DeMinter, J. R. Turner, D. Smith, R. A. Cary, 2004. Validation of a Semi-Continuous ECOC Instrument. *Atmospheric Environment*, 38, 2885-2893.
- 8) P. M. Fine, B. Chakrabarti, M. Krudysz, J. J. Schauer, and C. Sioutas, 2004. Seasonal, Spatial, and Diurnal Variations of Individual Organic Compound Constituents of Ultrafine and Accumulation Mode PM in the Los Angeles Basin. *Environmental Science and Technology*, 38, 1296-1304
- 9) S. C. Kerr, J. J. Schauer, and B. Rodger, 2004. Regional Haze in Wisconsin: Sources and the Spatial Distribution. *Journal of Environmental Engineering and Science*, 3, 213-222.
- 10) J. J. Schauer, G. C. Lough, W. C. Sonzogni, 2003, Outdoor Air Pollution Activities at the Wisconsin State Laboratory of Hygiene. *Wisconsin Medical Journal*, 102, 84-88.
- 11) C. Calhoun, C. S. Chistoforou, J. J. Schauer, 2003, PM<sub>2.5</sub> Characterization and Source-Receptor Relations in South Carolina. *Journal of Environmental Engineering and Science*, 2, 441-451.
- 12) J. J. Schauer, 2003. Elemental Carbon as a Tracer for Diesel Particulate Matter: A Review. *Journal of Exposure Assessment and Environmental Epidemiology*, 13, 443-453.
- 13) R. J. Sheesley, J. J. Schauer, J. D. Hemming, M. A. Barman, S. W. Geiss, and J. J. Tortorelli, 2003. Toxicity of Ambient Aerosols from the Lake Michigan Airshed to Aquatic Organisms. *Environmental Toxicology and Chemistry*, 23, 133-140.
- 14) P. Y. Chuang, R. M. DuVall, M. S. Bae, A. Jefferson, J. J. Schauer, H. Yang, J. Z. Yu, and J. Kim, 2003. Observations of Elemental Carbon and Absorption during ACE-Asia and Implications for Aerosol Radiative Properties and Climate Forcing. *Journal of Geophysical Research-Atmospheres*, 108, Article Number 8634.
- 15) S. S. Wong, N. N. Sun, I. Keith, C. B. Kweon, D. E. Foster, J. J. Schauer, M. W. Witten, 2003. Tachykinin Substance P Signaling Involved in Diesel Exhaust-Induced Bronchopulmonary Neurogenic Inflammation in Rats. *Archives of Toxicology*, 77, 638-650.
- 16) J. B. Manchester-Neesvig, J. J. Schauer, and G. R. Cass, 2003. The Distribution of Particle-Phase Organic Compounds in the Atmosphere and their Use for Source Apportionment during the Southern California Children's Health Study. *Journal of the Air and Waste Management Association*. 53, 1065-1079.
- 17) R. J. Sheesley, J. J. Schauer, Z. Chowdhury, G. R. Cass, B. R. T. Simoneit. 2003. Characterization of Organic Aerosols Emitted from the Combustion of Biomass Indigenous to South-Asia, 2003. *Journal of Geophysical Research-Atmospheres*, 108, D9, 4285-4299.

- 18) J. J. Schauer, B. T. Mader, J. T. DeMinter, G. Heidemann, M. S. Bae, J. H. Seinfeld, R. C. Flagan, R. A. Cary, D. Smith, B. J. Huebert, T. Bertram, S. Howell, P. Quinn, T. Bates, B. Turpin, H. J. Lim, J. Yu, and H. Yang, 2003. ACE-Asia Intercomparison of a Thermal Optical Method for the Determination of Particle-Phase Organic and Elemental Carbon. *Environmental Science and Technology*. 37, 993-1001.
- 19) B. T. Mader, J. J. Schauer, J. H. Seinfeld, R. C. Flagan, J. Z. Yu, H. Yang, H. J. Lim, B. J. Turpin, J. T. DeMinter, G. Heidemann, M. S. Bae, P. Quinn, T. Bates, D. J. Eatough, B. J. Hubert, and S. Howell, 2003. Sampling Methods Used for the Collection of Particle-Phase Organic and Elemental Carbon During ACE-Asia. *Atmospheric Environment*. 37, 1435-1449.
- 20) C. G. Nolte, J. J. Schauer, G. R. Cass, and B. R. T. Simoneit, 2002. Trimethylsilyl Derivatives of Organic Compounds in Source Samples and in Atmospheric Fine Particulate Matter. *Environmental Science and Technology*. 36, 4273-4281.
- 21) J. J. Schauer, M. P. Fraser, G. R. Cass, and B. R. T. Simoneit, 2002. Source Reconciliation of Atmospheric Gas-Phase and Particle-Phase Pollutants During a Severe Photochemical Smog Episode. *Environmental Science and Technology*. 36, 3806-3814.
- 22) M. D. Hays, C. D. Geron, K. J. Linna, N. D. Smith, and J. J. Schauer, 2002. Speciation of Gas-Phase and Fine Particle Emissions from Burning of Foliar Fuels. *Environmental Science and Technology*. 36, 2281-2297.
- 23) M. Zheng, G. R. Cass, J. J. Schauer, E. S. Edgerton, 2002. Source Apportionment of PM<sub>2.5</sub> in the Southeastern United States Using Solvent-Extractable Organic Compounds as Tracers. *Environmental Science and Technology*. 36, 2361-2371.
- 24) J. J. Schauer, M. J. Kleeman, G. R. Cass, and B. R. T. Simoneit, 2002. Measurement of Emissions from Air Pollution Sources. 5. C<sub>1</sub>-C<sub>32</sub> Organic Compounds from Gasoline-Powered Motor Vehicles. *Environmental Science and Technology*. 36, 1169-1180.
- 25) J. J. Schauer, M. J. Kleeman, G. R. Cass, and B. R. T. Simoneit, 2002. Measurement of Emissions from Air Pollution Sources. 4. C<sub>1</sub>-C<sub>27</sub> Organic Compounds from Cooking with Seed Oils. *Environmental Science and Technology*. 36, 567-575.
- 26) X. H. Song, N. M. Faber, P. K. Hopke, D. T. Suess, K. A. Prather, J. J. Schauer, and G. R. Cass, 2001. Source Apportionment of Gasoline and Diesel by Multivariate Calibration Based on Single Particle Mass Spectral Data. *Analytica Chimica Acta*. 446, 329-343.
- 27) C. G. Nolte, J. J. Schauer, G. R. Cass, and B. R. T. Simoneit, 2001. Highly Polar Organic Compounds Present in Wood Smoke and in the Ambient Atmosphere. *Environmental Science and Technology*. 35, 1912-1919.
- 28) J. J. Schauer, M. J. Kleeman, G. R. Cass, and B. R. T. Simoneit, 2001. Measurement of Emissions from Air Pollution Sources. 3. C<sub>1</sub>-C<sub>29</sub> Organic Compounds from Fireplace Combustion of Wood. *Environmental Science and Technology*. 35, 1716-1728.
- 29) J. J. Schauer and G. R. Cass, 2000. Source Apportionment of Wintertime Gas-Phase and Particle-Phase Air Pollutants Using Organic Compounds as Tracers. *Environmental Science and Technology*. 34, 1821-1832.
- 30) M. J. Kleeman, J. J. Schauer, and G. R. Cass, 2000. Size and Composition Distribution of Fine Particulate Matter Emitted from Motor Vehicles. *Environmental Science and Technology*. 34, 1132-1142.
- 31) M. P. Fraser, M. J. Kleeman, J. J. Schauer, and G. R. Cass, 2000. Modeling the Atmospheric Concentrations of Individual Gas-Phase and Particle-Phase Organic Compounds. *Environmental Science and Technology*. 34, 1302-1312.

- 32) M. J. Kleeman, J. J. Schauer, and G. R. Cass., 2000. Size and Composition Distribution of Fine Particulate Matter Emitted from Wood Burning, Meat Charbroiling, and Cigarettes. *Environmental Science and Technology*. 33, 3516-3523.
- 33) C. G. Nolte, J. J. Schauer, G. R. Cass, and B. R. T. Simoneit., 1999. Highly Polar Organic Compounds in Meat Smoke. *Environmental Science and Technology*. 33, 3313-3316.
- 34) J. J. Schauer, M. J. Kleeman, G. R. Cass, and B. R. T. Simoneit., 1999. Measurement of Emissions from Air Pollution Sources. 2. C<sub>1</sub>-C<sub>29</sub> Organic Compounds from Medium Duty Diesel Trucks. *Environmental Science and Technology*. 33, 1578-1587.
- 35) J. J. Schauer, M. J. Kleeman, G. R. Cass, and B. R. T. Simoneit., 1999. Measurement of Emissions from Air Pollution Sources. 1. C<sub>1</sub>-C<sub>29</sub> Organic Compounds from Meat Charbroiling. *Environmental Science Technology*. 33, 1566-1577.
- 36) B. R. T. Simoneit, J. J. Schauer, C. G. Nolte, D. R. Oros, V. O. Elias, M. P. Fraser, W. F. Rogge, and G. R. Cass., 1999. Levoglucosan, a Tracer for Cellulose in Biomass Burning and Atmospheric Particles. *Atmospheric Environment*. 33, 173-182.
- 37) J. J. Schauer, W. F. Rogge, L. M. Hildemann, M. A. Mazurek, G. R. Cass, and B. R. T. Simoneit., 1996. Source Apportionment of Airborne Particulate Matter Using Organic Compounds as Tracers. *Atmospheric Environment*. 30, 3837-3855.

#### Peer Reviewed Conference Proceedings

- 1) R. Ramakrishnan, J. J. Schauer, L. Chen, Z. Huang, M. M. Shafer, D. S. Gross, D. R. Musicant, "The EDAM Project: Mining Atmospheric Aerosol Datasets", International Journal of Intelligent Systems, Special Issue on KDD, 2004
- 2) Z. Huang, L. Chen, J. Y. Cai, D. Musicant, D. S. Gross, R. Ramakrishnan, J. J. Schauer, S. J. Wright, "Mass Spectra Labeling : Theory and Practice", ICDM, 2004
- 3) C. B. Kweon, S. Okada, J. C. Stetter, C. G. Christenson, M. M. Shafer, J. J. Schauer, D. E. Foster. 2003. Effect of Fuel Composition on Combustion and Detailed Chemical/Physical Characteristics of Diesel Exhaust. Society of Automotive Engineers (SAE) Paper 2003-01-1899.
- 4) C. B. Kweon, S. Okada, J. C. Stetter, C. G. Christenson, M. M. Shafer, J. J. Schauer, D. E. Foster. 2003. Effect of Injection Timing on Detailed Chemical Composition and Particulate Size Distribution of Diesel Exhaust. Society of Automotive Engineers (SAE) Paper 2003-01-1794.
- 5) C. B. Kweon, S. Okada, D. E. Foster, M. S. Bae, J. J. Schauer. 2003. Effect of Engine Operating Conditions on Particulate-Phase Organic Compounds in Engine Exhaust of a Heavy Duty Direct-Injection (D. I.) Diesel Engine. Society of Automotive Engineers (SAE) 2003-01-0342.
- 6) S. Okada, C. B. Kweon, J. C. Stetter, D. E. Foster, M. M. Shafer, C. G. Christensen, J. J. Schauer, A. M. Schmidt, A. M. Silverberg, D. S. Gross. 2003. Measurement of Trace Metal Composition in Diesel Engine Particulate and its Potential for Determining Oil Consumption. Society of Automotive Engineers (SAE) Paper 2003-01-0076.
- 7) C. B. Kweon, S. Okada, D. E. Foster, and J. J. Schauer. 2002. Detailed Chemical Composition and Particle Size Assessment of Diesel Engine Exhaust. Society of Automotive Engineers (SAE) Paper 2002-02FFL-180.



- 8) R. J. Sheesley, J. J. Schauer, N. D. Smith and M. D. Hays, 2000. Development of a Standardized Method for the Analysis of Organic Compounds Present In PM<sub>2.5</sub>. *Proceedings of 93<sup>rd</sup> A&WMA National Meeting*, Salt Lake City, Utah.
- 9) G. C. Lough, M. M. Shafer, J. J. Schauer, 2000. ICP-MS analysis of ultra-trace metals present in fine particulate matter. *Proceedings of 93<sup>rd</sup> A&WMA National Meeting*, Salt Lake City, Utah.

#### **Peer Reviewed Reports**

- 1) J. J. Schauer, G. C. Lough, M. M. Shafer, W. C. Christensen, M. F. Arndt, J. T. DeMinter, and J. S. Park. Characterization of Emission and Human Exposure to Metals Emitted from Motor Vehicles. Prepared for the Health Effect Institute (HEI) under a Research Agreement. 248 pages. In review.
- 2) J. J. Schauer and B. J. Turpin (2000) *Sources of Organic Particulate Matter: Composition and Source Tracers*. Prepared for US EPA as reference material for the US EPA Particulate Matter Criteria Document. 30 pages. Included in EPA Particulate Matter Criteria Document.
- 3) B. J. Turpin and J. J. Schauer (2000) *Organic Particulate Matter in the Atmosphere*. Prepared for US EPA as reference material for the US EPA Particulate Matter Criteria Document. 40 pages. Included in EPA Particulate Matter Criteria Document.



**ROBERT D. WILLIS, Ph.D.**  
**PRINCIPAL ENVIRONMENTAL SCIENTIST**

**EXPERIENCE SUMMARY**

- 28 years in environmental and applied physics research
- 13 years characterizing aerosols using electron microscopy and energy-dispersive x-ray analysis (SEM/EDX) and developing SEM/EDX methods for air pollution research
- 13 years in source apportionment and receptor modeling research
- 60 publications and 25 presentations

**EDUCATION:**

Ph.D., Physics, Duke University	1977
B.S. with Honors, Physics, Denison University	1970

**EMPLOYMENT HISTORY:**

ManTech Environmental Technology, Inc.	1992- present
Comstock, Inc., Oak Ridge, TN	August, 1991 - December, 1991
Atom Sciences, Inc., Oak Ridge, TN	1983-1991
Scripps Institution of Oceanography / Oak Ridge National Laboratory	1979-1983
Naval Research Laboratory, Washington, DC	1977-1979

**EXPERIENCE OVERVIEW:**

As Principal Environmental Scientist, provide support to the EPA in the areas of SEM methods development and applications, aerosol characterization, source apportionment and receptor modeling, and management and statistical analysis of air pollution data.

Operate and maintain the SEM Laboratory for EPA’s National Exposure Research Laboratory (NERL). Provide SEM/EDX characterization of aerosols in support of source apportionment research and human exposure studies. Conduct research to advance the state-of-the-art of SEM/EDX for the analysis of air particulates. Develop EPA guidance document for SEM/EDX analysis of air pollutants. Characterize size and chemistry of aerosols generated in EPA’s air particulate concentrator facility and develop SEM-based human exposure variables. Analyze air particulates using manual and automated SEM/EDX; design and conduct SEM data validation and quality assessment studies; provide assistance and training to outside users of the SEM facility; develop improved sample preparation methods and/or analysis protocols; supervise technician support; summarize and present analysis results to EPA customers.. Author or co-author of one EPA report and one journal publication in these areas.

Analyzed the Northern Front Range Air Quality Study (NFRAQS) using Chemical Mass Balance (CMB), Positive Matrix Factorization (PMF), and Unmix receptor models. Conducted data quality and receptor modeling analysis for COPPS (Car-Related Occupational Particulate Matter and Related Air Toxics Exposure to Patrol Troopers Study). As Co-PI on the Fort Hall Source Apportionment Study, collected and analyzed field samples; developed ambient air monitoring plan; conducted XRF and SEM analyses to identify contributing sources; applied receptor models to apportion sources; presented study findings to customer. Produced EPA document summarizing 2000 Workshop on UNMIX and PMF As Applied to

PM<sub>2.5</sub>. Conducted source-receptor modeling studies in the Czech Republic cities of Teplice and Ostrava and provided XRF and SEM analyses in support of the Czech study. Provided beta-testing for Chemical Mass Balance Receptor Model CMB8.0 and Unmix 3.0 and currently one of three consultants contracted by the EPA to peer review CMB8.2. Author or co-author on five publications and four technical reports in the above areas.

As Research Scientist, conducted research to characterize lead-bearing and pesticide-bearing dust in the environment. Characterized morphology and size-distribution of lead-rich particles in post-abatement house dust. Helped identify sources of children's exposure to lead in the CLEARs project (Childhood Lead Exposure Assessment Reduction Study). Determined the distribution of pesticides and PAHs in house dust as a function of particle size. Co-authored three publications in this area.

Prior to joining ManTech in 1992, Dr. Willis was PI on a Small Business Innovation Research (SBIR) grant to develop a novel laser-based IR spectrometer for measuring trace atmospheric gases (Comstock, Inc.). At Atom Sciences, Inc., Dr. Willis managed R&D activities culminating in a groundbreaking laser ionization time-of-flight facility for detecting noble gas isotopes with sub-ppt isotopic sensitivity; PI or Co-PI on \$1.7 million of R&D projects; researched applications of <sup>81</sup>Kr and <sup>85</sup>Kr as environmental tracers; trained and supervised technical staff; co-authored 11 publications. At Scripps Institution of Oceanography, Dr. Willis was Co-PI on a joint SIO-ORNL research program to develop an ultrasensitive, isotope-selective noble gas detector for oceanographic and environmental applications. At the Naval Research Laboratory, Dr. Willis designed and built an MeV ion microprobe and carried out novel microprobe studies investigating nitrogen-implanted materials.

Dr. Willis received ManTech Performance Incentive Program awards in 1993 and 1997 for his contributions to the Czech Project, and the President's Award in 2001 for the Fort Hall Source Apportionment Study.

#### **PUBLICATIONS:**

**Willis, R.D.**, F.T. Blanchard, and T.L. Conner. 2002. Guidelines for the application of SEM/EDX analytical techniques to particulate matter samples. U.S. Environmental Protection Agency (EPA). Office of Research and Development, Research Triangle Park, N.C., EPA 600/R-02/070

**Willis, R.D.**, W.D. Ellenson, and T.L. Conner. 2001. Monitoring and source apportionment of particulate matter near a large phosphorus production facility. *J. Air Waste Manage. Assoc.* 51:1142.

Mamane, Y., **R. Willis**, and T. Conner. 2001. Evaluation of computer-controlled scanning electron microscopy applied to an ambient urban aerosol sample. *Aerosol Sci. Technol.* 34:97.

**Willis, R.D.** 2000. Workshop on UNMIX and PMF as applied to PM<sub>2.5</sub>: final report. U.S. Environmental Protection Agency (EPA). Office of Research and Development, Research Triangle Park, N.C., EPA 600/A-00/048.

**Willis, R.D.** and W.D. Ellenson. 1999. Fort Hall source apportionment study: final report. U.S. Environmental Protection Agency (EPA). Office of Research and Development, Research Triangle Park, N.C., EPA 600/R-99/103.

Prahalad, A.K., J. Soukup, J.I. Inmon, **R. Willis**, A. Ghio, S. Becker, and J. Gallagher. 1999. Ambient air particles: effect on cellular oxidant radical generation in relation to particulate elemental chemistry. *Toxicology and Applied Pharmacology* 158:81.

Lewis, R.G., C.R. Fortune, **R.D. Willis**, D.E. Camann, and J.T. Antley. 1999. Distribution of pesticides and polycyclic aromatic hydrocarbons in house dust as a function of particle size. *Environmental Health Perspect* 107:721.

Pinto, J., R. Stevens, **R. Willis**, Y. Mamane, J. Novak, J. Santroch, I. Benes, J. Lenicek, P. Subert, V. Bures, and R. Kellogg. 1998. Czech air quality monitoring and receptor modeling study. *Environ. Sci. & Tech.* 32:843.

Adgate, J.L., **R.D. Willis**, T.J. Buckley, J.C. Chow, J.G. Watson, G.G. Rhoads, and P.J. Lioy. 1998. Chemical mass balance source apportionment of lead in house dust. *Environ. Sci. & Tech.* 32:108.

Ellenson, W.D., S. Mukerjee, R.K. Stevens, **R.D. Willis**, D.S. Shadwick, M.C. Somerville, and R.G. Lewis. 1997. An environmental scoping study in the lower Rio Grande Valley of Texas. Part II: Assessment of transboundary pollution transport and other activities by air quality monitoring. *Environment International.* 23:643.

Mukerjee, S., W.D. Ellenson, R.G. Lewis, R.K. Stevens, M.C. Somerville, D.S. Shadwick, and **R.D. Willis**. 1997. An environmental scoping study in the lower Rio Grande Valley of Texas. Part III: Residential microenvironmental monitoring for air, house dust, and soil. *Environment International.* 23:657.

**Willis, R.D.**, W.D. Ellenson, J.P. Pinto, T.A. Hartlage, J. Novak, J. Dostalek, L. Cernikovsky, and V. Bures. 1997. Ostrava air quality monitoring and receptor modeling study. U.S. Environmental Protection Agency (EPA). Office of Research and Development, Research Triangle Park, N.C., EPA/600/R-97/030.

Wang, E., **R.D. Willis**, T.J. Buckley, G.G. Rhoads, and P.J. Lioy. 1996. The relationship between the dust lead concentration and the particle sizes of household dusts collected in Jersey City residences. *J. Applied Occupational and Environmental Hygiene.* 11:199.

Mukerjee, S., M.C. Somerville, **R.D. Willis**, D.L. Fox, R.K. Stevens, R.B. Kellogg, D.C. Stiles, T. A. Lumpkin, and C. M. Shy. 1996. Integrated assessment of reduced emission impacts from a biomedical waste incinerator. Atmospheric characterization and modeling applications on particulate matter and acid gases. *Environ. Sci. & Tech.* 30:1680.

Stevens, R.K., J.P. Pinto, **R.D. Willis**, Y. Mamane, J. Novak, I. Benes, and J. Lenicek. 1995. Monitoring and modeling of air pollution in the Czech Republic. In: *Proceedings of the Second International Symposium on Environmental Contamination in Central and Eastern Europe.* Budapest, Hungary.

Stevens, R.K., J.P. Pinto, **R.D. Willis**, Y. Mamane, J.J. Novak, and I. Benes. 1995. Monitoring and modeling methods for developing air pollution control strategies: a case study in the northwest Czech Republic. In: *Proceedings of the NATO Advanced Research Workshop on Urban Air Pollution.* Erice, Italy.

Mamane, Y., **R.D. Willis**, R.K. Stevens, and J.L. Miller. 1995. Scanning electron microscopy/X-ray fluorescence characterization of lead-rich post-abatement dust. In: M. Beard and S. Iske, eds. *Lead in*

*Paint, Soil, and Dust: Health Risks, Exposure Studies, Control Measures, Measurement Methods, and Quality Assurance* (ASTM STP 1226), 268. Philadelphia, PA: American Society for Testing and Materials.

Conner, T.L., J.L. Miller, **R.D. Willis**, R.B. Kellogg, and T.F. Dann. 1993. Source apportionment of fine and coarse particles in southern Ontario, Canada. Paper 93-TP-58.05. In: *Proceedings of the 86th Annual Meeting of the Air & Waste Management Association*. Pittsburgh, PA: Air & Waste Management Association.

Stevens, R.K., J.P. Pinto, T.L. Conner, **R.D. Willis**, R.A. Rasmussen, Y. Mamane, G. Casuccio, I. Benes, J. Lenicek, P. Subrt, J. Novak, and J. Santroch. 1993. Czech Air Toxic Study (CATS) Project Summary. Paper 93-RA-138A.03. In: *Proceedings of the 86th Annual Meeting of the Air & Waste Management Association*. Pittsburgh, PA: Air & Waste Management Association.

Thonnard, N., M.C. Wright, W.A. Davis, and **R.D. Willis**. 1992. The second-generation RIS-TOF noble gas detector: Detection limits below 100 atoms in less than 5 minutes. *Resonance Ionization Spectroscopy 1992* (Inst. Phys. Conf. Ser. 128:27). Bristol: Institute of Physics.

**Willis, R.D.**, N. Thonnard, O. Eugster, Th. Michel, and B.E. Lehmann. 1991. The cosmic-ray exposure age of the Millbillillie meteorite determined by conventional mass spectrometry and by RIS-TOF. In: J.E. Parks and N. Omenetto, eds. *Resonance Ionization Spectroscopy 1990* (Inst. Phys. Conf. Ser. 114), 275. Bristol: Institute of Physics.

Thonnard, N., H.F. Arlinghaus, **R.D. Willis**, E.H. Taylor, M.C. Wright, W.A. Davis, M.T. Spaar, and L.J. Moore. 1991. The status of real-world analysis problem-solving using RIS. In: J.E. Parks and N. Omenetto, eds. *Resonance Ionization Spectroscopy 1990* (Inst. Phys. Conf. Ser. 114), 271. Bristol: Institute of Physics.

Lehmann, B.E., H.H. Loosli, D. Rauber, N. Thonnard, and **R.D. Willis**. 1990. Krypton-81 and Krypton-85 in a water sample from the Milk River aquifer (Canada). *J. Appl. Geochem.* Special volume on Milk River.

**Willis, R.D.**, N. Thonnard, M.C. Wright, B.E. Lehmann, and D.F. Rauber. 1989. Counting  $^{81}\text{Kr}$  atoms in groundwater using RIS-TOF. In: T.B. Lucatorto and J.E. Parks, eds. *Resonance Ionization Spectroscopy 1988* (Inst. Phys. Conf. Ser. 94), 213. Bristol: Institute of Physics.

Thonnard, N., J.E. Parks, **R.D. Willis**, L.J. Moore, and H.F. Arlinghaus. 1989. Resonance ionization of neutral atoms with applications to surface science, noble gas detection and biomedical analysis. *Surf. Interface Anal.* 14:751.

**Willis, R.D.**, N. Thonnard, and D.R. Cole. 1989. Resonance ionization spectroscopy and its potential application in geosciences. *Bull. U.S. Geol. Surv.* 1890:117.

Thonnard, N., **R.D. Willis**, M.C. Wright, W.A. Davis, and B.E. Lehmann. 1987. Noble gas atom counting using RIS and TOF mass spectrometry II: First results. In: G.S. Hurst and C.G. Morgan, eds. *Resonance Ionization Spectroscopy 86* (Inst. Phys. Conf. Ser. 84), 75. Bristol: Institute of Physics.

- Lehmann, B.E., D.F. Rauber, N. Thonnard, and **R.D. Willis**. 1987. The challenge of sorting out 1000 atoms of Krypton-81 from  $10^{25}$  molecules of water. In: G.S. Hurst and C.G. Morgan, eds. *Resonance Ionization Spectroscopy 86* (Inst. Phys. Conf. Ser. 84), 81. Bristol: Institute of Physics.
- Lehmann, B.E., D.F. Rauber, N. Thonnard, and **R.D. Willis**. 1987. An isotope separator for small noble gas samples. *Nucl. Instrum. Methods Phys. Res.* B28:571.
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PROFESSIONAL EXPERIENCE

**Data Analyst 2000-present**

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Analyze air quality data from multiple networks to derive relationships between air quality parameters, meteorological parameters, and emissions. Determine the sources of pollutants and meteorological conditions associated with good and poor air quality. Develop and apply statistical models (CMB, CART, regression, variance components). Plan and implement field studies and special monitoring projects. Review existing monitoring networks.

**Environmental Scientist 1996-2000**

*U. S. Environmental Protection Agency Chicago, IL*

Oversaw the collection of air quality data from the Photochemical Assessment and Monitoring Stations, performed statistical analyses of data from various air quality monitoring networks, and examined emission inventories for consistency with ambient data. Worked closely with state, regional, and national monitoring community to coordinate data analyses and disseminate results. Planned and managed short-term air sampling projects for research and investigations.

**Research Specialist 1989-1996**

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Research focus encompassed (1) receptor modeling of VOCs to determine the relative contributions of industrial sources to ambient air pollution and (2) application of these results to urban ozone modeling to develop ozone control curves. Analyzed data from the Lake Michigan Ozone Study and the Southeast Michigan Ozone Study.

**Policy Analyst, Technical Editor 1980-1989**

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## SELECTED PUBLICATIONS AND PRESENTATIONS

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**APPENDIX D**

**INDIVIDUAL REVIEWER'S COMMENTS**

**EPA-EPA-CMB8.2 Peer Review**  
**Review Comments by Jamie Schauer**  
**Nov 27, 2004**

Introduction

The following comments concerning the review of EPA-CMB8.2 were based on a review of the two manuals<sup>a</sup> provided with the EPA-CMB8.2 software and running the EPA-CMB8.2 software on two computers. The EPA-CMB8.2 software was run with both input files provided by the EPA and by input files created specifically for the review testing. The review was conducted in a manner that was intended to assess the usability of the manuals and software by researchers, engineering, and regulators working in the air quality and public health fields. The review was performed in a manner that assumed that the user would have prior experience with CMB modeling but did assume that the user had moderately proficient in computer skills and assumed that the user would be applying the EPA-CMB8.2 software with reasonable understanding of air quality issues and the role of receptor based air quality modeling in understanding and regulating air quality problems. The review did not specifically attempt to find operating conditions that would make the EPA-CMB8.2 software fail but rather pursued a strategy to operate the model over reasonable conditions that would be expected by typical users from the research, engineering, regulatory and public health fields. Software errors that were found to be corrected by restarting the EPA-CMB8.2 software or were not reproducible were assumed to be associated with the computer operating system and are not reported as part of the review.

<sup>a</sup> The two manuals provided with the review are as follows:

EPA-CMB8.2 Users Manual, September 2004

Protocol for Applying and Validating the CMB Model for PM<sub>2.5</sub> and VOC

Overall Assessment

EPA-CMB8.2 is significant improvement over previous version of EPA's CMB software releases. EPA-CMB8.2 effectively takes advantages of the Windows<sup>®</sup> operating systems, which allows users to efficiently create input files, efficiently operate the model, and efficiently review and analyze the model results within the framework of the software and through software output files. Relative to other air quality modeling software and other specialized technical software, EPA-CMB8.2 is very user friendly

and flexible to meet the broad needs of the air quality field. The manuals provide a solid foundation on the appropriate use of the EPA-CMB8.2 and the theoretical and statistical basis for the model, as well as excellent reference lists for CMB users who need additional information. The CMB input files provided with the model provide an excellent training tool for new users and provide an ideal reference for users that are developing new input files. Although the software and the accompanying documentation are currently in suitable form for use by the research, engineering, regulatory and health effects community, there are certainly opportunities to improve the software and associated documentation. The following critiques highlight the opportunities to improve the software and documentation to make the model more effectively and efficiently used by the intended audience.

### Comments on Software

#### *General Comments*

1. The biggest problem with the model is the error messages that are associated with errors that arise from non-EPA-CMB8.2 software. These error messages are typically due to input file formatting problems that are often very difficult to diagnose. Although the EPA-CMB8.2 software has a series of checks that provide well described and documented error messages, many formatting problems with the input files are not identified by the EPA-CMB8.2 software that ultimately lead to software errors that provide cryptic descriptions that yield frustration for the user. Although it seems impractical for EPA to revise EPA-CMB8.2 to catch all of these potential errors, EPA should consider the possibility of developing a simple, format checking software that could read in all of the CMB 8.2 input files and check formatting and data framework consistencies. This would make a huge contribution toward trouble shooting of EPA-CMB8.2.
2. The MIDAS.DLL files had to be installed before the EPA-CMB8.2 software would run properly. This is not currently addressed in the manuals and is not currently provided with the EPA-CMB8.2 software and should be addressed before the final version of the manuals and software is released.
3. EPA should be commended for providing five complete sets of EPA-CMB8.2 input files for the user to test and review. However, it is concerning that some of these data sets and the associated project reports were never published in the peer reviewed scientific literature. Clearly, EPA's intention in providing these data sets is to support EPA-CMB8.2 modeling operations and not to provide key studies as references for CMB modeling. Nonetheless, at the least one of these non-

peer reviewed studies is highly controversial and has a significant impact on the scientific communities assessment of CMB modeling, much of which is expected to arise in the peer reviewed literature in the next 2-5 years. It is important to recognize that one of the key intended uses of EPA-CMB8.2 is to support development of SIPs, which will be highly scrutinized by the public and private sector. It would be unfortunate, if state agencies use the controversial non-peer reviewed study as a key reference for the development of the CMB efforts that would be used in the development of a SIP. For this reason, EPA should strongly consider replacing the CMB files from non-peer reviewed studies with files from peer-reviewed that would provide better references for EPA-CMB8.2 users. As a minimum, the report should explicitly state that EPA does not intend these provided files or associated reports to be a guideline in CMB analysis but rather examples and guidelines for EPA-CMB8.2 software operations.

4. A problem was identified regarding the operation of the EPA-EPA-CMB8.2 model without a run file (i.e. the manual selection of input files). This mode has some major flaws that make the model inoperable and the user should use this mode with caution. The most significant problem observed with this mode is the shifting and/or misalignment with labels during interactive use of the source profile and species selection windows.

The following describes the scenario where the problem has occurred during testing of the software;

- Run the SJV test case without a control file;
- Load \*.CSV files for the AD and PR file;
- Load the three \*.sel files, individually;
- Do not change anything and run the model – Note the results;
- Move to the “Species” page and do the following;
  - Click on array 3
  - Star (\*) nitrate
  - Click on array 1
  - Remove the \* for sulfate, which has now moved to the top of the list
  - Click on array 3
  - Click back on array 1
  - Star (\*) sulfate, which is now at the bottom of the list
- The order of the species is now different but all of the species in array 1 are the same as the original run
- Rerun the model and the results are different.

### *Specific Comments*

1. On the *Options* page of the EPA-CMB8.2, the spinners only allow the iteration delta, the minimum source uncertainty, and the decimal places to span from 0-20, 0-100, and 1-6, but these numbers can be changed manually to wider ranges without an error message. Some of these conditions, including some erroneous values, will allow the model to run and others will yield an error during the model run. The minimum source projection does not allow values to be entered manually that go beyond the specified control limits. The iteration delta, the minimum source uncertainty, and the decimal places should be modified to follow the constraints limiting manual entries.
2. The pop-up help icon for “decimal places displayed” on the *Options* page appears to contain the wrong information.

### Comments on the *EPA-CMB8.2 User’s Manual*

#### *General Comments*

1. More explanation of the Britt-Luecke algorithm testing needs to be presented on page 3-5 and X-Y. It is unclear if the insufficient testing is for the EPA-EPA-CMB8.2 software code or the application to CMB calculations. Although the manual provides adequate precautions, the user should understand the precautions better.
2. More discussion on the appropriate use of source elimination is needed on page 3-5 and page 6-2. The user should be warned that they should not just use source elimination as a starting point. Proper CMB analysis requires an understanding of why sources are being removed. The removal of a source for colinearity purposes is not the same as removal due to negative but not statistically significant source contributions. In addition, removal of sources without removal of tracers can often lead to violation of source completeness for specific tracers.
3. Section 4, pages 4-1 through 4-13: It would be helpful to the user to add a paragraph about units and EPA-EPA-CMB8.2. Although there are common units that are frequently used in EPA-EPA-CMB8.2, the software is actually very flexible. The output units are equal to the units used in AD\* divided by the units in PR\*. This provides considerable flexibility for the model. This is specifically relevant to the second to last paragraph on page 4-10.

4. Section 4, pages 4-1 through 4-9: Clearly, one of the most frustrating aspects of setting up the CMB input files is finding errors in formatting and codes that are inconsistent across files and ultimately make the model fail. A convenient strategy to avoid such problems is to start with only AD\* and Pr\* files and let the software make the three \*.sel files but loading these two files and then saving the three \*.sel files. This will require adding text and asterisks to these files but can avoid many careless errors associated with setting up these files. This strategy should be offered to the user in this section.
5. Section 6.1.1, pages 6-2 through 6-3. The basis for the acceptable criteria for R-square and chi-square needs to be provided. In addition, the C/M ratios should be added as performance criteria. In addition, the statement that percent mass should be in the range of 80% to 120% is not a fair criteria. I model can be very accurate, even exact, if some sources are missing from the model AND the missing sources are not contributors to the fitting species. I perfect example if the absence of secondary inorganic species from a CMB model.
6. Section 6.1.2, pages 6-4 through 6-5: More discussion on the appropriate setting for maximum source uncertainty and minimum source projection is needed. In several places in the manual, it is stated that hard-wired CMB7 values were appropriate for PM that used XRF data but that these values are not appropriate for VOC data and presumable other analytical methods. As a minimum, some recommendations should be offered for VOC data. In addition, the implication of changing these values needs to be presented.
7. Appendix G: The information about the EST parameter needs to be moved to the main body of the manual. The implication of the “lack of understanding of the EST parameter” on selection of source elimination needs to be discussed as well.
8. In the context of General Comment 3 under the Comments on Software, it is bothersome that the “Protocol for validating the CMB Model for PM<sub>2.5</sub> and VOC” relies so heavily on the NFRAQS study. It is important to note that the NFRAQS study is very controversial and has not been published in the peer reviewed literature. The results of this study are very controversial and are not general excepted being validated by the scientific community. This manual contains a lot of good information but is undermined the use of this study as the example of validation for PM CMB.

### *Specific Comments*



1. Page 2-3, lines 2-7. It would helpful to the reader to explain briefly at this point what the different files are used for.
2. Pages 3-2 through 3-3: Although the manual explains in details the differences between using an in\*.in8 files later in the manual, it would be helpful to the reader to add one or two sentences at this point in the manual that explain the differences of operating with the in\*.in8 and not using this files.
3. Page 3-4, bottom half of the page: The acceptable ranges for iteration delta, maximum source uncertainty, and minimum source projections should be added here to aid the user.
4. Page 3-6 – The discussion of the help icon and Figure 3-5 should be moved to an earlier section of the manual.
5. Page 3-17 – It would be good to add a brief explanation of the “forward”, “back”, “start”, “end”, “save”, and “print” icons that appear on the top of the screen whent EPA-EPA-CMB8.2 is running.
6. Page 4-7, line 3: the column number for the asterisk should column 36 as noted several lines down on this page.
7. Page 4-11, email from John Watson: This material is very confusion and the presentation of this material as an email from John Watson is an awkward mechanism to reference the material.
8. Pages 5-1 through 5-9: The term “VCR control buttons” needs to be better defined or explained. It is possible to annotate these buttons with a label on Figures 5.2 through 5.7.
9. Page 5-9, last paragraph. In the reviewed version of the SJV files, the comments were not missing for the subject profiles.
10. Page 6-1, lines 3 – The EPA (2001) reference is missing from the list of references. Is this really the second manual?
11. Page 6-8, lines 6-7: The statement that a poor fit for a CMB model should motivate efforts to find a profile that would fit better with the data is not good advice. Source profiles should be picked because they are meaningful and not because they fit the data. Given enough source profiles many good fits can be found that clearly will provide a wrong answer.

## Review of CMB8.2

Bob Willis

January 15, 2005

### Documentation

1. The **Manual**: I think the contents and organization of the Manual are quite good, and I think documentation is sufficient to guide a typical user through the application of the model. There are some errors/typos/confusions in the manual which are highlighted in the hardcopy and/or listed below under Manual Errors.
2. The **Protocol**: The Protocol contains a wealth of valuable and practical information, but needs editing for grammar, typos and clarity. I think the contents and organization of the Protocol are adequate. I'm glad to see the NFRAQS and NARSTO studies discussed in such detail, although sometimes I felt that the NFRAQS discussion got bogged down by perhaps too much detail (page 5-16), though perhaps the protocol requires it. But it's important to show how the CMB protocol is applied and validated in actual field studies, and I think Chapters 5 and 6 provide a valuable service in this regard. Recommended changes and/or correction for the Protocol are listed below.
3. I think the Protocol appendices are useful. See annotations on pages B-5 and G-4 for possible errors. In Table G-1, the summed species abundances in the AMSUL and AMBSULF profiles exceed 1. Is this allowed? Appendices E and F summarize PM10 and VOC source apportionment studies, respectively, using two different formats. (1) I think they should both use the same format, and my preference is the Appendix F format, although I certainly appreciate that this represents a major effort. (2) I think Appendix E should be broadened to include PM2.5 and PM coarse studies. As Appendix E now stands, one of the model CMB applications, NFRAQS, is excluded because it was a PM2.5 study. [And, the Protocol, after all, is specifically directed toward PM2.5 and VOC applications, although I don't see why it shouldn't be more broadly targeted to PM and VOC applications]. (3) It seems that the last studies included in Appendices E and F may date back to 1996. Are there more recent CMB studies that need to be included? Again, I think these suggestions would improve the Protocol but I also know that these changes would require considerable effort.

### Performance Evaluation

With minor exceptions, the SJVF test case behaved as described in the manual. There were some errors in the Manual or deviations from the Manual related to the test data set which are annotated in the Manual or discussed below.

Other data sets were tested with the model to test for program stability, errors, and aberrant behavior. Recommendations for future development or frustrations experienced with the model are listed below. The following software bugs were identified.

### **Software Bugs:**

Most of the software bugs listed below, while potentially frustrating, don't lead to erroneous results and can be dealt with as time and money permit. Items 7, 9, and 14, however, require fixing in my opinion before the program can be released. Bugs 9 and 14 have the potential to generate erroneous results, and 7 is a must-fix flaw affecting the operation of the program. Item 12, which could frustrate many users, might be relatively easy to fix. I would guess that items 5 and 6 are carryovers from the previous version of CMB.

1. Start CMB with a control file and go to Input Files. If you delete an input file and try to replace it using the Browse button, browse will not work. (Browse will work if you replace the existing filename without first deleting it. On the other hand, if you do not use a control file, Browse works fine to load input filenames in the empty boxes.) Manually typing in the filename however, seems to work.
2. Related bug: if I create a copy of one of the input files, give it a different name, then try to replace the original input file with its copy, Information Box pops up with message saying the copy may be incompatible with the PR\* file directed by the Control File ...
3. Create a control file without an optional AD selection file. Start CMB. Info box says to supply AD\*.sel file to initialize sample selection. If you manually type in selection file then run CMB, the selection file is ignored. Using Browse to enter the selection file seems to work.
4. Problem running with self-created control file. Example: Start CMB with no control file. Use Browse function to fill in supplied sjvf.\* files (ADsjvf.txt, PRsjvf.txt, SPsjvf.sel, and PRsjvf.sel). Save new control file as INsjvf.test. Exit CMB and restart using INsjvf.test control file. Information screen pops up with message that the optional ambient data selection file does not exist. Click Ok.

- Click on Options, or Samples, or Species Tab. C++ Debug Library screen pops up with message “Debug assertion failed!” There is no way out except to abort CMB.
5. Calculated fit measures do not agree with the formula on page 6-10 of the manual. You can see what the program is doing by successively zeroing all weights but one and re-running a fit. The Fit Measure is correct when Rsq and %Mass are the only weighted parameters. The FM is a factor of 2 in error when  $\chi^2$  is the only weighted parameter, and FM goes bonkers when Fraction Estimate is the only weighted parameter. (I got a FM of 9999!)
  6. I believe the FM formula on page 6-10 of the manual is wrong, aside from the question of what is the correct weighting for  $\chi^2$ . Shouldn't the entire expression be divided by a normalization factor equal to the sum of the weights? (I believe the FM as calculated in the program is normalized, but the equation in the manual is missing the normalization factor).
  7. If you modify a species or source array within CMB, then highlight the modified array (or any other array) or run a fit, the changed species or source is moved to the bottom of the arrays. For example, modify species array #1. Now perform a fit with the modified array. The species used in the fit are the same as those selected in array 1, but if you examine array1, the changed species is now at the bottom of the array. Now click on array 1. Nothing changes visibly with array 1, but if you repeat the fit, the fitting species have changed! And if you select any other species array and perform a fit, the actual fitting species are different from what the array shows as being selected. And if you save the selection file after performing a fit, the saved file is screwed up.
  8. Run CMB with control file INsjvf.in8. Select source array 3 and species array 3. Try to fit sample 3. I get error message suggesting that something is wrong with the fitting sources. But source array 3 will give fits using the other 3 species arrays, so the problem seems to be, at least in part, with the species array.
  9. CSV and TXT output files are not identical in the last two columns, and both are missing data. Example: run CMB with INsjvf.in8 control file. Run. File, Save current record only as \*.txt file. Now, go to Options and select \*.csv output format. Run. File, Save current record only as \*.csv file. Compare .txt and .csv files in Excel. They differ in the last two columns. The csv file has column headings but no data for SJV065 and Soil 31. The txt file has neither data nor column headings for this source. This source was unselected in the selection file. However, selecting this source and re-running the results as before makes no difference: both output files are missing data for this last source. And I echo Donna's question of why include data for the unselected sources?
  10. Data box which accompanies the graphs of sources or samples won't display all species if you have a large number of species. Should there be a scroll button?

11. Missing data (-99.) in source profiles or ambient data show up numerically as -99 in View Graph plots. Is this your intention? It effectively renders the graph useless for the other species.
12. Modifying and saving an AD\*.sel file does not work: the modified selection file puts the \* one column to the left of where it needs to be. But there seems to be a more subtle problem as well. Example: load INNfraqs.in8 control file. (No AD\*.sel file is included). Select all samples and save \*.sel file. Exit CMB and restart. Load new AD\*.sel file and look at the samples: none are selected. Looking at the \*.sel file in Notepad, the \* are one column left of where they should be. Using Notepad, shift all the \* one column to the right and re-run CMB. Only those samples with a start time of '06' are selected. What's going on?
13. No control file was provided for the COAST test data. I tried running CMB with both the \*.DBF and \*.txt input files but got error messages each time: Number of tokens in the PR input file does not equal number of tokens in the header.
14. I think there is a bug in either the calculation or the display of source projections. They appear to be inconsistent, at least at times, with the identification (YES or NO) that a source is estimable. Example: Load the NFRAQS control file. Select Bright sample 12/25/96, start time 0600. Source N010 is identified as non-estimable, yet its source projection is listed as 0.9987, greater than the 0.95 threshold for an estimable source; sources N050 and N084 are listed as estimable but their source projections are both considerably less than 0.95.
15. I got the following error message when I tried running my own data set: "A component named SIZE already exists". The problem was that my AD and PR files both had columns named "size" in lower case. I had to rename the columns in all caps (SIZE) in order to get CMB to run. Example: using Notepad, modify the NFRAQS AD and PR data files, changing the heading "SIZE" to "size" and rerun CMB. If you do the same modification to the San Joaquin AD and PR files you get the error message: "A component named SID already exists".
16. This last item is not a bug, but an observation that may merit a suggestion to the user in the manual for accelerating batch processing of large data sets. When CMB processes multiple samples, CMB scrolls every result through the results window with a subsequent loss of speed. To accelerate the calculations, one can bypass the scrolling (after about the third cycle) and make the program go into "turbo mode" by clicking on the File & Help taskbar until the message "Not Responding" appears in the frame bar. This significantly speeds up the calculations. Example: running all 205 San Joaquin samples on my laptop took 76 seconds in the normal mode versus 29 seconds in the "turbo mode". Try it! Why shouldn't the program always run in the "turbo" mode? Nothing is gained by watching the results scroll by in the results window.

**Errors in the Manual:**

1. Page v: Sections 3.3 and 3.4 appear on pages 3-7 and 3-8, respectively.
2. P. vi: Figure 4.1 appears on P.4-3, not 4-4.
3. P.1-5, 2<sup>nd</sup> Par: “corrects of model..”?
4. P.2-2, 2<sup>nd</sup> bullet: PACS.zip or Portland.zip?
5. P.2-2, last line: \test case\ not \text case\.
6. P.3-6, first line: ..values between 0 and 1 (not 10,000)
7. P.3-11: PR appears twice. Shouldn’t these instead be SP\* and AD\*, respectively?
8. P.3-12: Is Figure 3.9 really what you meant to show as the “results screen”?
9. P.4-1 and 4-2: On p.4-1 manual states that input files can have any 8-character file name. On p.4-2, bottom paragraph, it states that extended file names may be used. ???
10. P.4-5, 4-10 and 5-9 (final paragraph): I found no ill consequences if the source mnemonics in the \*.sel and PR\*.txt input files are different: the source asterisk and comment fields are not affected. The ill consequences warned of in the manual occur when the source codes (first fields) differ in the two input files.
11. P.5-6, last sentence: the header file displays 6 (not 0) samples, and a look back at the sample array shows that the samples originally selected are still selected: they have not been De-selected.
12. P6-4: Instead of the shown display, I think it would be more instructive to show the eligible space display for a sample for which there are collinearities, so that the manual could discuss (last paragraph of p.6-5) an actual example of estimable linear combinations of inestimable sources.
13. P6-4: Section 6.1.2 has some redundancies and could be tightened up.
14. There is some confusion about the Std Err when TSTAT <1. Page 6-2 of the manual, 1<sup>st</sup> paragraph states: “Two or three times the SE may be taken as an upper limit of the source contributions..” However, Table 4.2-1 of the Protocol in discussing the SE states: “When the SCE is less than the SE, the SE is interpreted as an upper limit of the source contribution.”

See notations in manual for other corrections.

**Complaints/Recommendations for Future Development:**

1. Something basic to help the user select fitting species would be nice. E.g., the program could show, for each species, the mean ambient concentration, the percent of observations exceeding the uncertainty, the average signal to noise ratio, and a correlation matrix for ambient species. Sure, it

- could be done outside the CMB program using Excel or other software, but I think many users would appreciate it.
2. One cannot overestimate the importance of good, quality-assured input data. Any aides to help the user eliminate bad data and select good fitting species I think might be useful to the average user. The Manual might include a discussion on how to deal with missing data values or values below the detection limit. (E.g., replacing sub-MDL data with  $1/2 * MDL$ , or replacing missing values if possible by regression against another species with which the missing species is highly correlated). Also, perhaps some guidance on eliminating outlier data – either in individual ambient concentrations or entire ambient observations.
  3. Having to click in each individual cell to change the selections in the sample, species, and source arrays is cumbersome –It should be made more efficient so that one can highlight many cells at once and select or de-select all with one click. Also, it would make life easier in setting up multiple species arrays if one could copy and paste an existing array into a new array (providing a starting array which is then much easier to modify).
  4. How about flagging those fits where the calculated mass falls outside  $\pm 20\%$  of the measured mass? I think unacceptable solutions should be distinguished from those which predict mass more accurately.
  5. It would be convenient if CMB would recognize tab-delimited text input files, as this seems to be the default text format for Excel. I believe Unmix automatically recognizes what delimiter is used and accepts both space- and tab-delimited text files as well as .xls files. CMB should do the same.
  6. Source and AD bar graphs are a welcome addition. However, they become unreadable for a large number of species. Perhaps one needs an option to only plot selected species?
  7. In the batch mode, a useful option might be to show and/or print only a subset of the solutions which meet user-specified criteria – e.g.,  $R^2 > 0.8$ ,  $\chi^2 < 1$ , and %Mass within  $\pm 20\%$  of measured mass.
  8. Best Fit is not as useful as it could be. It fits only paired species and source arrays. Given 10 species arrays and 10 source arrays, Best Fit only fits 10 out of 100 possible combinations. Although this is explained in the manual, unsophisticated users at some time will mistakenly assume that their Best Fit is the best of all possible combinations.
  9. Rather than just show the single Best Fit, have an option so show the top 5 or top 10 Best Fits.
  10. An Abort Run button would be nice to stop the program (without exiting) in the middle of unwanted calculations.



11. When viewing the source or samples arrays, it would be nice to be able to highlight the entire row of data for a selected source or sample, so that as you scroll to the right to view data you can be sure you are on the right row.
12. What happened to some of the graphical output that was part of the original CMB8 such as time-series bar charts and source contribution pie charts? Also, “Present Computed Averages” is gone. I thought these were useful features.
13. I think it would be nice to be able to change the default options (e.g., number of iterations) so that they can be preserved from one session to another.
14. Some error messages are cryptic and not very helpful. Example: “Column (source) Number [] of Afit = 0.” Could you instead say “Source xxx has zero concentrations for all species. Change the source profile or remove the source”? Another example: “AKT\*VeffIn\*AK matrix needs improvement...”. Can you say instead: “Two or more sources are probably collinear. Change fitting sources or fitting species to remove the collinearity”? Also, if some error messages are potentially misleading, can’t they be changed to be more helpful? [See my notes attached to pages F-5 and F-8 of the manual].
15. Eventually, I would hope that CMB will have enough built-in intelligence to troubleshoot bad fits. For example, if the %MASS is <80% and one or more species have R/U ratios << -2, the software should someday be able to examine the source profiles and suggest additional profiles to try that might supply the missing mass.

#### **Errors or Items Needing Clarification in the Protocol:**

1. See hardcopy editorial notations for many grammar and typo errors.
2. Sec. 5.7 starts by stating that CMB8 source contribution estimates for carbon are consistent with other NFRAQS data analysis and simulations. Immediately after this, the reader learns that the CMB results at Welby predict a gas to diesel source contribution ratio that is much larger (inconsistent with) the emission inventory (Table 5.1-1). These two statements seem contradictory.
3. Can the possible heavy hydrocarbon artifact mentioned with respect to Fig. 6.7-2 be elucidated at all? Did the other sites show the same, relatively non-directional source contribution for diesel exhaust? If it’s a sampling artifact, why did it occur at only the Lynn site (if indeed it did)? According to Fig. 6.7-2, it appears that diesel exhaust was typically the largest source – and to have to discount the largest VOC contributor as a sampling artifact seems to be a serious accusation which doesn’t inspire confidence in the diesel contribution estimates at the other sites. Hopefully,



the results at Lynn were an aberration rather than representative of NARSTO and this should be clarified for the reader.

4. Figure 6.7-1 appears to be missing plots for the LPG and CNG source contributions.
5. Sec. 4.3.7: In the discussion of corroborating CMB results with other modeling and analyses, dispersion modeling is recommended. I think there should also be some mention of multivariate receptor models such as Unmix, PMF, and Factor Analysis (if the data permit) as additional ways to confirm CMB results or provide consistency checks.
6. Sec. 5: Actual CMB results are only presented for the Welby site (a pie chart of SCEs), but not the Brighton site. Was there a reason to exclude Brighton results? Was CMB less successful with the Brighton data, and if so, would there be some value in including the Brighton results as an example of challenges posed by some data sets?
7. Sec. 6: The actual NARSTO CMB apportionment results are never shown, though they are discussed. I think a table summarizing the CMB fits to the ambient data should be included. The text in Sec. 6.6 states that there is “good agreement between calculated source contributions and measured ambient concentrations...”. But I’d like to see the results first hand and confirm that conclusion.
8. When summarizing CMB results – e.g., presenting average source contributions over the duration of the study – is there an accepted procedure for dealing with CMB fits that fail to meet the target fit parameters? For example, do you discard any fits that miss the measured mass by more than 20%, even though  $R_{sq}$  and  $Ch_{sq}$  are acceptable? Does the protocol address this question?

## CMB Review Comments

**Donna Kenski**

General: Overall, CMB8.2 is a big improvement over previous versions. The current documentation is very thorough and exhaustively detailed, so the comments that follow are minor. The graphical interface is clean and reasonably intuitive. The one major drawback remains the balky process of building a set of input files that CMB8.2 will accept. Once the files are acceptable to the program, running them seems to go smoothly and without major glitches; the few error messages that cropped up were simple to deal with.

I ran the program with the supplied datasets (most extensively with the \*SJF files, although I exercised the others a bit) and some of my own making. The supplied datasets worked exactly as described in the manual. My own did not, although eventually they were beaten into submission; this process was ultimately quite revealing and led to some of the specific comments below.

Specific: Sec. 3.4: Add a note here (in the first ¶, after the sentence “Within a given array...”) that says something like “Species within a given array can only be added or removed if the array has been previously highlighted by clicking on the index number.”

Sec. 3.5: The comment field in the Fitting Sources Array screen (as shown in Fig. 3.8) is truncated, even if you expand the field using the sliders. I.e., even though you make the comment field wider, the comments don’t seem to refresh, so the ends of each are cut off.

Sec. 4.2.1, last ¶: The underlined sentence doesn’t seem to be consistent with the rest of the ¶. If you don’t use a control file, why should it matter what directory the (nonexistent) control file is in?

Section 4.2.2 : The order in which the detailed file descriptions are given would be better if you started with the ambient data file, then the source profile file, then the selection files, then the control file. I never bothered with the selection files; they seem like an unnecessary step, especially since CMB is so fussy about formatting details. It was so tedious to build the source profile and ambient data files that it didn’t seem worth the extra work to build selection files, when the selection options are built into CMB and can be saved as files anyway.

Sec. 4.2.3: The names of the variables are apparently more restricted than the manual indicates here, in length and characters allowed. The manual needs to be more specific about exactly what variable names are supported.

Sec. 4.2.4: Must the *order* of species and species variability in this file be identical to the order of the same variables in the ambient data file? The manual clearly states that the names must be identical, but doesn't say anything about the order.

This section should include additional clarification on the units of variability; from the test data sets, it looks like they are expressed in mass fraction, but I couldn't find this stated explicitly. The actual units really shouldn't matter so much, as long as the files are internally consistent – this could be pointed out in the text with an example. The email citation from Watson is a little odd; can't this be incorporated into the text without the blue color and reference? It's not clear why the definitions of Fields 11 and 12 are in red – they don't seem to have any emphasis in the text.

(??) It's awkward to have to close CMB to switch files. This may be more of an issue in testing than in actually running CMB (although it is bound to happen frequently when constructing a data set that is acceptable to CMB) but nevertheless it was an annoyance. Also, once you exit, you can't cancel out of the exit; you're prompted to save files but not to cancel the actual exit, so if you make a mistake you're stuck.

Section 5: The use of the test data sets supplied with CMB worked just as promised, with no detectable glitches. The manual was very thorough and the step-by-step series of instructions made the process very clear. The screen shots were very helpful.

The 'Main Report' screen should add a line that describes the meaning of the < symbols after the measured and calculated values (at the bottom of the report where the species concentrations are listed). This is described in Section 6.1.3, but it would probably be more useful (at least easier to find) if it were moved up to Sec. 5.

The 'Contributions by Species' screen could use some additional clarification; I'd suggest adding another line or two to the actual output to indicate that the values in the source columns are fractions of the measured mass. This is described in the text but not within the program. Also, if you happen to include a

fitting species that has a zero source contribution from all sources, the source contribution in this screen comes out as -9.9; it should be zero. (Has anyone else encountered this?)

The meanings of column headings for the output file are not immediately obvious. An example, with descriptions, should be added to the manual, perhaps in Section 5 or alternatively, in Section 4.3.2. At least add a note in Section 5 explaining that the output file is described in detail in 4.3.2. If possible, it would be helpful to rename the estimate and uncertainty headings to the profile names and profile uncertainties, rather than the current profile number and profile name. Also, why are non-fitting profiles included in the output file? This makes the file unnecessarily big and unwieldy.

Sec. 7, References: This is very picky, but in a reference list only the first author's name should be inverted, not all but the last (see, for example, the Chicago Manual of Style). So the first reference is okay (Anderson et al.) but the next multiple-author listing (Belsley, Kuh, and Welsch) should be Belsley, D.A., E. Kuh, and R.E. Welsch. The reference list in the protocol is done correctly.

Equations A-10, A-12: I don't know if "I" should be bolded or not, but this question should be deleted from the text :)

Appendixes B-D: I did not review this because I don't have any knowledge of these codes.