CHEMICAL MASS BALANCE RECEPTOR MODEL VERSION 8 (CMB8) USER'S MANUAL

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Abstract

The Chemical Mass Balance (CMB) air quality model is one of several receptor models that have been applied to air resources management. CMB8 is a Windows 95 based version of CMB modeling software that substantially facilitates the estimation of source contributions to specieated PM_{10} (particles with aerodynamic diameters less than 10 µm), $PM_{2.5}$ (particles with aerodynamic diameters less than 2.5 µm), and Volatile Organic Compound (VOC) data sets. This manual introduces CMB8 and its development history. It describes minimal and desired hardware and software requirements and shows how to install CMB8 on a personal computer. It explains CMB8 menu options and input and output file formats. The manual provides a step-by step tutorial of CMB8 operations using the example data sets provided with the model. Performance measures are briefly described, though their use in practical applications is deferred to a separate applications and validation protocol. A significant bibliography of CMB-related literature is included for those desiring more information about the CMB, its utility and applications.

Acknowledgements

CMB8 software has been under development since 1995 and has benefited from beta testing since 1996 by many users from all over the world who are too numerous to identify here. Further suggestions are welcome from other users, and can be directed to Norman Robinson at normr@sage.dri.edu. Norman Mankim and Mary MacLaran of DRI's staff provided publications support for the production and distribution of this manual and the compilation of references.

Table of Contents

1.   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 mechanisms 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.

This manual describes how to operate CMB Version 8 (CMB8) modeling software to calculate source contributions to ambient PM_{10} (particles with aerodynamic diameters less than 10 µm), $PM_{2.5}$ (particles with aerodynamic diameters less than 2.5 µm), and Volatile Organic Compounds (VOCs).

A separate applications and validation protocol (Watson et al., 1998) describes how to apply CMB8 to specific situations and how to evaluate its outputs. Several review articles, books, and conference proceedings provide additional information about the CMB and other receptor models (Chow et al., 1993; Gordon, 1980, 1988; Hopke and Dattner, 1982 ; Hopke, 1985, 1991; Pace, 1986, 1991; Stevens and Pace, 1984; Watson, 1979; 1984, 1989, 1990, 1991).

1.1   CMB8 Features

CMB8 replaces CMB7 (U.S. EPA, 1989; Watson et al., 1990) as a more convenient method of estimating contributions from different sources to ambient chemical concentrations. CMB8 returns the same results of CMB7, but it operates in a Windows-base environment and accepts inputs and creates outputs in a wider variety of formats than CMB7. The major CMB8 enhancements are:

- **Windows-based, menu-driven operations:** CMB commands may be executed with hot-keys, drop down menus, or toolbar buttons.

- **Multiple defaults for fitting source, fitting species, and sample selection:** Up to ten combinations of fitting source profiles and fitting species may be specified in input data selection files. Different defaults can be selected with radio buttons during CMB8 operation. Subsets of source profiles, species, and samples may be specified in selection files to be selected from profile and ambient concentration data files.

- **Improved memory management:** CMB8 memory is limited only by the available RAM on the computer, not by pre-set memory limitations.

- **Flexible input and output formats:** Comma-separate value (CSV), xBASE (DBF), and worksheet (WKS) formats are support as input and output files, in addition to the blank-delimited ASCII text files (TXT) supported by CMB7.

- **Improved graphics:** Sample pie plots, spatial pie plots, time series stacked bar charts, source profile bar charts, and ambient concentration bar charts can be created within CMB8. These can be cut from their CMB8 windows and pasted into other Windows documents.

- **Improved collinearity diagnostics:** The uncertainty/similarity clusters have been replaced with an singular value composition eligible space treatment that allows the user to define an acceptable error and an acceptable collinearity among weighted source profiles.

- **Automatic decision-making:** CMB8 calculations can be automated to eliminate negative contributions and to select a default set of profiles based on a weighted optimization of performance measures.

- **User-set preferences:** Output directories, output file names, positions of decimal points in output, output formats, automatic calculation alternatives, performance measure weights, eligible space tolerances, receptor concentration units, and maximum iterations for convergence can be set by the user.

- **Retention from previous sessions:** Options and window position preferences established in one session are carried over into subsequent sessions.

CMB8 differs from CMB7 in the following:

- CMB8 no longer supports CMB6 style ambient data and source profile data files.

- Filename, source profile, ambient data, and sample selection file formats differ slightly from CMB7. CMB7 source profile and ambient concentration data files can be read directly by CMB8, however, so backward compatibility is assured.

- Graphical output is no longer provided as HPGL text files. Instead output can be printed through Windows or copied to the clipboard for insertion into documents. Text output can also be directed to the printer, the clipboard, or a report file.

1.2 Chemical Mass Balance Overview

The CMB receptor model (Friedlander, 1973; Cooper and Watson, 1980; Gordon, 1980, 1988; Watson, 1984; Watson et al., 1984; 1990; 1991; Hidy and Venkataraman, 1996) consists of a solution to linear equations that express each receptor chemical concentration as a linear sum of products of source profile abundances and source contributions. The source profile abundances (i.e., the mass fraction of a chemical or other property in the emissions from each source type) and the receptor concentrations, with appropriate uncertainty estimates, serve as input data to the CMB model. The output consists of the amount contributed by each source type represented by a profile to the total mass and each chemical species. The CMB calculates values for the contributions from each source and the uncertainties of those values. The CMB is applicable to

multi-species data sets, the most common of which are chemically-characterized PM_{10} (suspended particles with aerodynamic diameters less than 10 µm), $PM_{2.5}$ (suspended particles with aerodynamic diameters less than 2.5 µm), and VOC (Volatile Organic Compounds).

The CMB modeling procedure requires: 1) identification of the contributing sources types; 2) selection of chemical species or other properties to be included in the calculation; 3) estimation of the fraction of each of the chemical species which is contained in each source type (source profiles); 4) estimation of the uncertainty in both ambient concentrations and source profiles; and 5) solution of the chemical mass balance equations. The CMB is implicit in all factor analysis and multiple linear regression models that intend to quantitatively estimate source contributions (Watson, 1984). These models attempt to derive source profiles from the covariation in space and/or time of many different samples of atmospheric constituents that originate in different sources. These profiles are then used in a CMB to quantify source contributions to each ambient sample.

Several solutions methods have been proposed for the CMB equations: 1) single unique species to represent each source (tracer solution) (Miller et al., 1972); 2) linear programming solution (Hougland, 1973); 3) ordinary weighted least squares, weighting only by precisions of ambient measurements (Friedlander, 1973; Gartrell and Friedlander,1975); 4) ridge regression weighted least squares (Williamson and DuBose, 1983); 5) partial least squares (Larson and Vong, 1989; Vong et al., 1988); 6) neural networks (Song and Hopke,1996); and 7) effective variance weighted least squares (Watson et al., 1984).

The effective variance weighted solution is almost universally applied because it: 1) theoretically yields the most likely solutions to the CMB equations, providing model assumptions are met; 2) uses all available chemical measurements, not just so-called "tracer" species; 3) analytically estimates the uncertainty of the source contributions based on precisions of both the ambient concentrations and source profiles; and 4) gives greater influence to chemical species with higher precisions in both the source and receptor measurements than to species with lower precisions. The effective variance is a simplification of a more exact, but less practical, generalized least squares solution proposed by Britt and Luecke (1973)

CMB model assumptions are: 1) compositions of source emissions are constant over the period of ambient and source sampling; 2) chemical species do not react with each other (i.e., they add linearly); 3) all sources with a potential for contributing to the receptor have been identified and have had their emissions characterized; 4) the number of sources or source categories is less than or equal to the number of species; 5) the source profiles are linearly independent of each other; and 6) measurement uncertainties are random, uncorrelated, and normally distributed.

The degree to which these assumptions are met in applications depends to a large extent on the particle and gas properties measured at source and receptor. CMB model performance is examined generically, by applying analytical and randomized testing methods, and specifically for each application by following an applications and validation protocol. The six assumptions are fairly restrictive and they will never be totally complied with in actual practice. Fortunately, the CMB model can tolerate reasonable deviations from these assumptions, though these deviations

increase the stated uncertainties of the source contribution estimates (Cheng and Hopke, 1989; Currie et al., 1984; deCesar et al., 1985, 1986; Dzubay et al., 1984; Gordon et al., 1981; Henry, 1982, 1992; Javitz and Watson, 1986; Javitz et al., 1988a, 1988b; Kim and Henry,1989; Lowenthal et al., 1987, 1988a, 1988b, 1988c, 1992, 1994; Watson, 1979).

The formalized protocol for CMB model application and validation (Pace and Watson, 1987; Watson et al., 1991; 1998) is applicable to the apportionment of gaseous organic compounds and particles (Watson et al., 1994a; Fujita et al., 1994). This seven-step protocol: 1) determines model applicability; 2) selects a variety of profiles to represent identified contributors; 3) evaluates model outputs and performance measures; 4) identifies and evaluates deviations from model assumptions; 5) identifies and corrects of model input deficiencies; 6) verifies consistency and stability of source contribution estimates; and 7) evaluates CMB results with respect to other data analysis and source assessment methods.

The CMB is intended to complement rather than replace other data analysis and modeling methods. The CMB explains observations that have already been taken, but it does not predict the future. When source contributions are proportional to emissions, as they often are for PM and VOCs, then a source-specific proportional rollback (Barth, 1970; Cass and McCrae, 1981; Chang and Weinstock, 1975; deNevers, 1975) is used to estimate the effects of emissions reductions. Similarly, when a secondary compound apportioned by CMB is known to be limited by a certain precursor, a proportional rollback is used on the controlling precursor. The most widespread use of CMB over the past decade has been to justify emissions reduction measures in PM_{10} non-attainment areas. More recently, the CMB has been coupled with extinction efficiency receptor models (Lowenthal et al., 1994; Watson and Chow, 1994) to estimated source contributions to light extinction and with aerosol equilibrium models (Watson et al., 1994b) to estimate the effects of ammonia and oxides of nitrogen emissions reductions on secondary nitrates.

The CMB model does not explicitly treat profiles that change between source and receptor. Most applications use source profiles measured at the source, with at most dilution to ambient temperatures and <1 minute of aging prior to collection to allow for condensation and rapid transformation. Profiles have been "aged" prior to submission to the CMB using aerosol and gas chemistry models to simulate changes between source and receptor (Friedlander, 1981; Lin and Milford, 1994; Venkatraman and Friedlander, 1994). These models are often overly simplified, and require additional assumptions regarding chemical mechanisms, relative transformation and deposition rates, mixing volumes, and transport times.

The CMB model requires species with different abundances in different source types, and abundances that do not vary by more than approximately ±100% among source types. The consistency of a species abundance is more important than the uniqueness for source quantification. The uniqueness is useful to identify which sources to include in a CMB. Combining particle and gas properties for source emissions, normalized to NMHC (non-methan hydrocarbon) or $PM_{2.5}$ mass emissions, could assist the apportionment of both VOCs and $PM_{2.5}$.

New analytical methods, however, such as isotopic abundances, specific organic compounds, and single particle morphology may be used in the CMB when they have been

applied to source and receptor samples to more precisely differentiate among contributions from different sub-types. The CMB performs tests on ambient data and source profiles that tell how well source-type contributions can be resolved from each other for different combinations of source profiles and chemical measurements.

The CMB model quantifies contributions from chemically distinct source-types rather than contributions from individual emitters. Sources with similar chemical and physical properties cannot be distinguished from each other by the CMB. The CMB model calculates source contribution estimates for each individual ambient sample. The combination of source profiles that best explains the ambient measurements may differ from one sample to the next owing to differences in emission rates (e.g., some days may have wood-stove burning bans in effect and others will not), wind directions (e.g., a downwind point source would not be expected to be contributing at an upwind sampling site), and changes in emissions compositions (e.g., different gasoline characteristics and engine performance in winter and summer may result in different profiles).

1.3   CMB Software History

The Chemical Mass Balance (CMB) receptor model was first applied by Winchester and Nifong (1971), Hidy and Friedlander (1972), and Kneip et al. (1972). 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 are typically much higher than the uncertainties of the receptor concentrations, were neglected.

The first user-oriented software for the CMB model 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. CMB7 was completely rewritten in a combination of the C and FORTRAN languages to operate on microcomputers with floating-point coprocessors, hard disk systems with tens of megabytes storage, and available memory of 640 kilobytes. CMB8 upgrades the DOS character-based CMB7 to a Windows graphical user interface through the use of the programming language Delphi. Source code is in the public domain and is available for modification.

1.4   Organization of User's Manual

Section 1 introduces CMB8 and the scope of this manual. Section 2 describes minimal and desired hardware and software requirements and shows how to install CMB8 on a personal computer. Section 3 describes CMB8 menu options while Section 4 documents input and output file formats. Section 5 provides a step-by step tutorial of CMB8 operations using the example

data sets provided with the model. Performance measures are briefly described in Section 6, though their use in practical applications is deferred to a separate document (Watson et al., 1998). Section 7 includes a bibliography of CMB-related literature, including references cited throughout this software manual.

2.   SOFTWARE INSTALLATION

This section describes the hardware requirements, computer programs, and installation procedures for CMB8.

2.1   Hardware and Operating System

The minimum requirements for running CMB8 software are:

- IBM PC compatible desktop, portable, or laptop computer with 386 processor and 8 MB RAM

- Hard disk drive with 100 MegaBytes

- MS Windows 3.1 or higher operating system

The recommended hardware configuration is:

- IBM compatible Intel Pentium microcomputer with 32 MB of RAM.

- Super VGA video graphics adapter and monitor.

- Graphics capable printer.

- Windows 95 or Windows NT operating system.

2.2   CMB Software

CMB8 software can be acquired from the National Technical Information Service or it can be retrieved from the EPA's Support Center For Regulatory Air Models Bulletin Board System (SCRAM BBS), or the EPA's FTP site

ttnftp.rtpnc.epa.gov:/e-drive/scram/cmb8/

The following files are available and can be downloaded as needed:

- **CMB832.EXE:** A self-extracting compressed file containing the executable CMB code and supporting windows files for 32-bit operating systems. This includes all applications using Windows 95 and Windows 3.1 that have been upgraded to 32-bit processing. This is the file that should be downloaded unless one is using an older, and currently unsupported, 16-bit Windows 3.1 operating system.

- **CMB816.EXE:** A self-extracting compressed file with the same contents as CMB832.ZIP except that it operates on Windows 3.1 16-bit operating systems. This version is included only for backward compatibility. Most users do not need this file.

- **CMB8MAN.EXE:** A self-extracting compressed file containing an Adobe Acrobat (CMB8MAN..PDF) file and Microsoft Word 97 (CMBDOC?.DOC) files of this User's Manual. Use this manual to learn CMB8 features and operating methods.

- **CMB8DPOR.EXE:** A self-extracting compressed file of the example PM_{10} data in Portland, OR, from the Portland Aerosol Characterization Study (Watson et al., 1979) used to demonstrate basic CMB8 model features in this manual. This example is identical to that used for CMB7.

- **CMB8DSJV.EXE:** A self-extracting compressed file of example $PM_{2.5}$ data from several sites in California's San Joaquin Valley Air Quality Study (VAQS, Chow et al., 1990; 1992) that is used in the example application in Section 5 of this manual.

- **CMBDNAR.EXE:** A self-extracting compressed file of example hydrocarbon canister data in Boston, MA, from the North American Regional Study of Tropospheric Ozone (NARSTO) VOC source apportionment in Boston, MA (Fujita et al., 1997) that shows how files can be set up for VOC canister measurements.

- **CMBDHOU.EXE:** A self-extracting compressed file of example continuous (hourly) hydrocarbon measurements in Houston, TX, from the Coastal Oxidants Atmospheric Study (Fujita et al., 1995).

- **CMB8SOR.EXE:** A self-extracting compressed file of CMB source code. This file preserves the source code for further updates and allows it to be inspected for scientific verification. Most users do not need this file. CMB8 software is written in the C, FORTRAN, and Delphi computer languages. The executable files are produced using compilers from Borland (Delphi), Watcom (16 bit C and FORTRAN), and Microsoft (32 bit C and FORTRAN).

The examples given in this manual are specific to the Windows 95 installation and use of the 32-bit software. These examples can be followed for Windows 95 or the installation of the 16-bit software, though the illustrated displays will appear different.

2.3   Installing CMB8 Software

Create a folder entitled CMB80 and transfer the CMB832.EXE file into the folder. Double-click the mouse on the CMB832.EXE icon and the needed software will self-extract to create the operations files, as shown in Figure 2.3.1. The other compressed files for test data sets and instructions can be also be obtained by double-clicking on the appropriate icon. icons. The *.DLL and other executable files that accompany CMB8.EXE must be present in the same directory for the program to properly execute.

The most convenient way to start CMB8 is to open the CMB8 folder and double-click on the CMB8 icon. CMB8 may also be installed by using the Add/Remove Program utility on the Windows 95 Control Panel. It can also be added to the Windows 95 Start Menu by clicking the

Start/Settings/Taskbar utility and selecting the CMB80/CMB8.exe program. After this is completed, CMB8 can be started from the Start/Programs Menu. A desktop or toolbar shortcut can also be created by following standard the Windows 95 procedures.
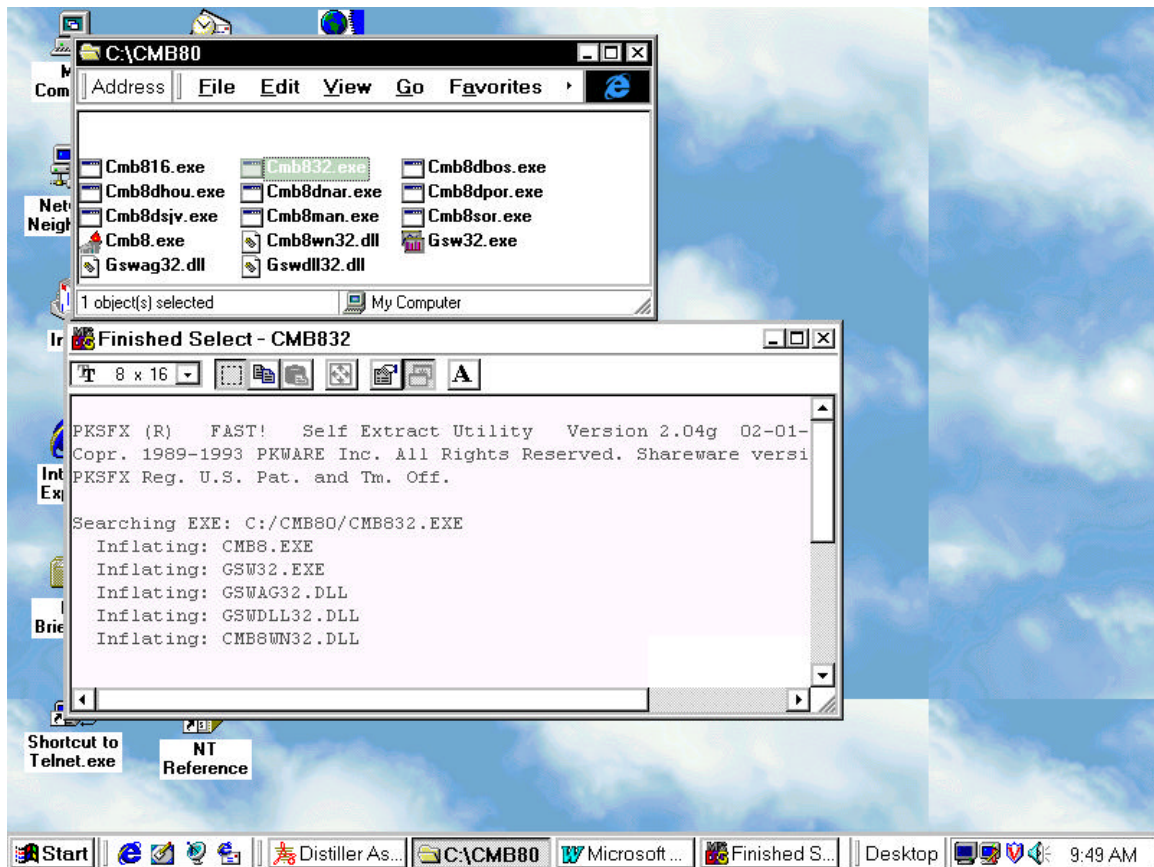
Figure 2.3.1. Installing CMB8 software.

3. CMB8 COMMANDS

This section describes the CMB model commands. The appearance of example screens may differ slightly from those seen during an actual application owing to differences in hardware and software configurations.

CMB8 commands can be selected from drop down menus, the tool bar, or by using keyboard shortcuts. The 3-letter mnemonic is supplemented by a reminder when the cursor in placed over the button. Below the tool bar is a status bar where the currently selected ambient data record is displayed and an indication of whether a fit has been done on the currently selected ambient data record is displayed.

3.1 File Menu Commands

Figure 3.1.1 shows the File menu options that are accessed by clicking on the File mnemonic with the mouse arrow. ALT-F can also be used to access this menu using the keyboard. Keyboard shortcuts for all menu items are underlined.
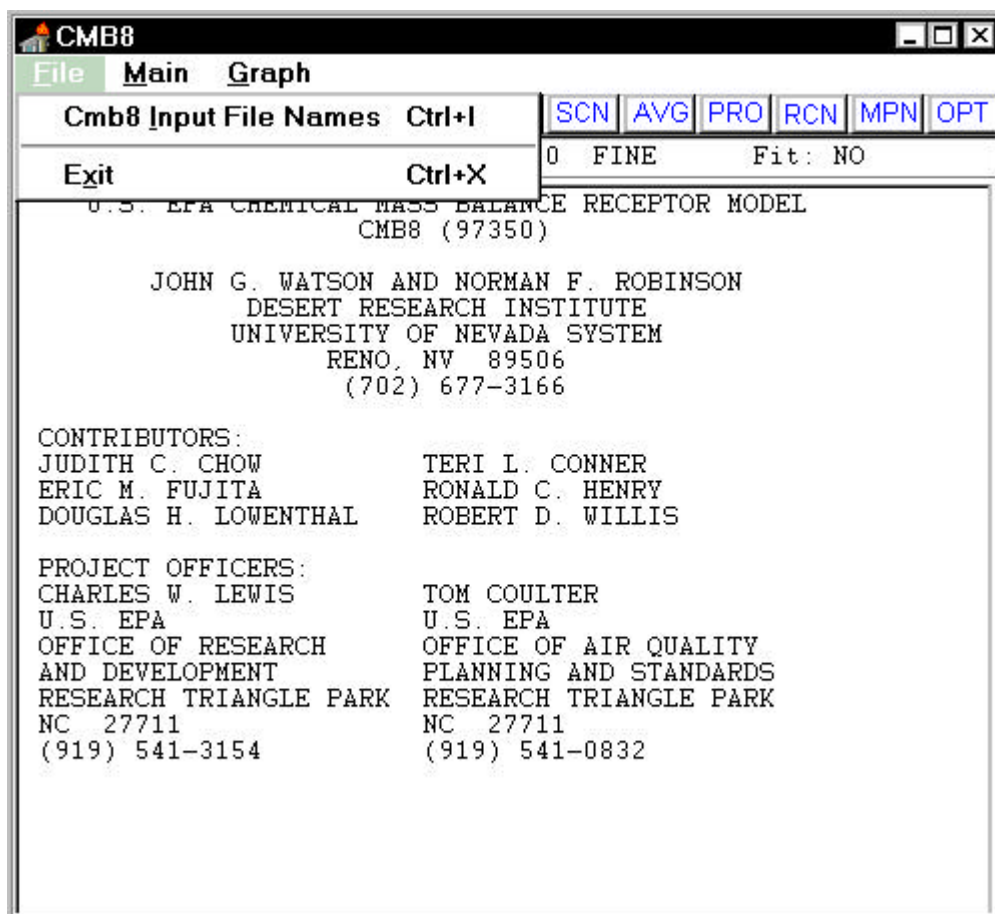
Figure 3.1.1. File menu options.

The file menu options are:

- **CMB8 Input File Names (CTRL-I):** Selection of this item brings up a window for selection of a input file names file. The function of this file is identical to that of the input file names file prompted for upon program invocation, and this menu item may be used to start a new session without the need to exit and restart the program.

- **Exit (CTRL-X):** Selection of this item terminates the program.

3.2 Main Menu Commands

The main menu, shown in Figure 3.2.2 contains the commands that are most commonly used to perform CMB calculations and evaluate performance.
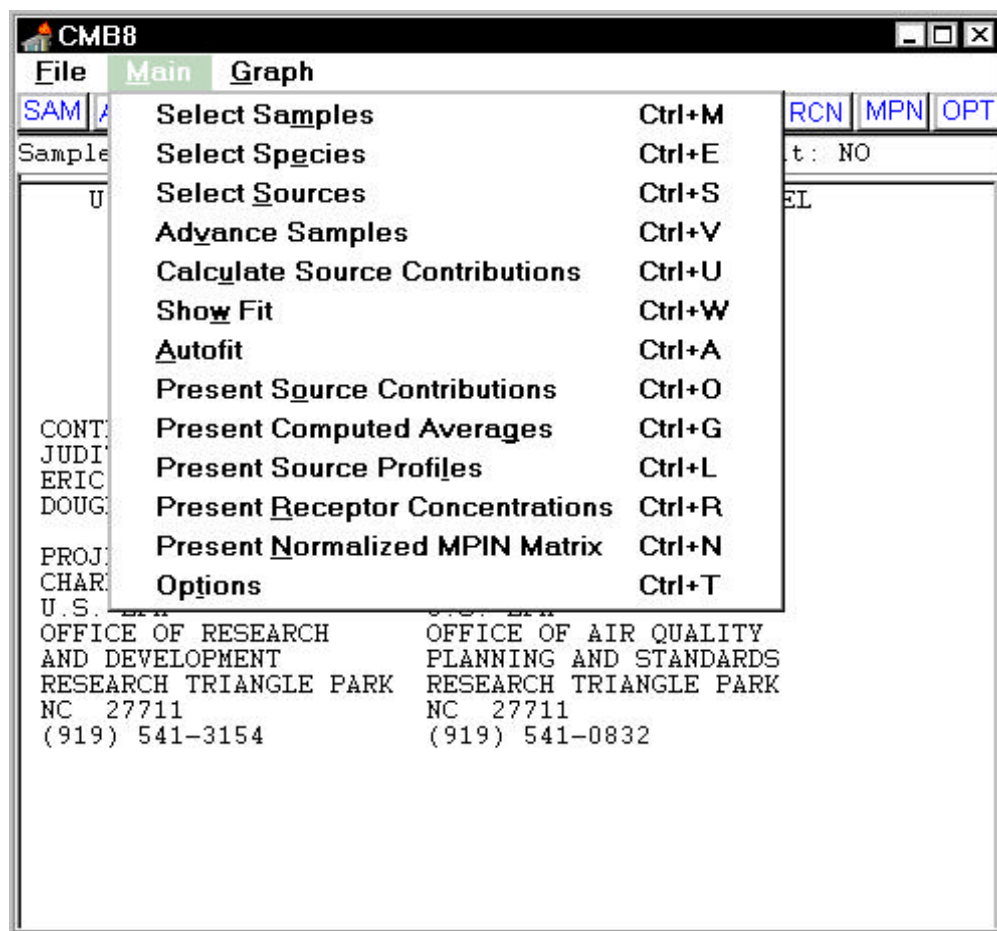
Figure 3.2.1. Main menu options.

These commands are described below with their shortcut keys and Toolbar buttons.

- **Select Samples (SAM, CTRL-M):** The sub-set of samples on which CMB source apportionments will be performed is selected by this command. Select or deselect an ambient data record by clicking on the desired ambient data record item. Selection is

indicated by the presence of the asterisk. Click the Select All or Deselect All button to select or deselect all samples, respectively.   Click the OK button to record the selection and deactivate the menu; the sample selection menu must be deactivated to progress further with the program. Upon leaving this menu the first selected ambient data record is defined to be the current ambient data record and CMB fits are performed on it. The sample selection window, as well as other windows, may be moved to other locations on the desktop.

- **Select Species (SPE, CTRL-E):** Fitting species are used in the calculation of source contribution estimates. Species not included in this calculation are termed floating species. The comparison of calculated and measured values for floating species is part of the model validation process. Fitting species should be selected that are major or unique components of the source-types influencing the receptor concentrations. Default fitting   species are selected in the species selection input file (e.g. PO????.SEL) and are indicated by an asterisk next to the species name. The Select All or Deselect All buttons designate all or none of available choices as fitting species. Click on an individual species mnemonic to select or deselect it, as indicated by the presence or absence of an asterisk. This window may be left open during a CMB session and can be resized and moved to a convenient location on the Windows desktop. Click the Close button to remove it. Click the Defaults button to select from up to ten different combinations of fitting species specified in species selection input file. Click the Modify button to modify any of the default selections. Click the OK button to deactivate the defaults window, which is required for further progress.

- **Select Sources (SRC, CTRL-S):** Fitting source profiles are included in the CMB calculation and are selected to represent the emissions most likely to influence receptor concentrations.. Several profiles may be available that represent the same source-type, but only one of these is usually used as a fitting source. Profiles of similar chemical composition are often found to be collinear when two or more are selected as fitting sources. Default fitting species are selected in the profile selection input file (e.g. SO????.SEL) and are indicated by an asterisk next to the source mnemonic. The Select All or Deselect All buttons designate all or none of available choices as fitting sources. Click on an individual source mnemonic to select or deselect it, as indicated by the presence or absence of an asterisk. This window may be left open during a CMB session and can be resized and moved to a convenient location on the Windows desktop. Click the Close button to remove it. Click the Defaults button to select from up to ten different combinations of fitting sources specified in profile selection input file. Click the Modify button to modify any of the default selections. Click the OK button to deactivate the defaults window, which is required for further progress.

- **Advance Samples (ADV, CTRL-V):** This action retrieves data from the next sample in the sample selection list. It is used after a satisfactory CMB calculation has been completed and the results recorded. Note that the sample identification information below the toolbar changes to identify the current sample being analyzed.

- **Calculate Source Contributions (FIT, CTRL-U):** This action performs the least-squares estimation of source contribution estimates and performance measures on the selected sample data using the designated fitting species and source profiles. Of note is the way CMB8 handles missing values in source and receptor files (designated by –99 in place of the value). When a fitting species value is missing in CMB8, that species is automatically removed from the calculation and the species selection flat is set to "M" in the report output file. If this procedure results in more fitting sources than fitting species an error message is written, and all fitting sources and calculated species are set to missing values. The FIT command causes source contribution estimates and performance measures to appear in the output window.

- **Show Fit (SHO, CTRL-W):** This command displays output from the most recent CMB calculation in the output window. This is useful for reviewing results after the window has been cleared. The contents of the output window can also be selected with the left mouse button and copied from pop-up menu that appears when the right mouse button is clicked. The output window can be sized and re-located on the Windows desktop where it will appear in the current and subsequent sessions. Several toolbar buttons appear at the bottom of the output window that perform various functions as shown in Figure 3.2.2.
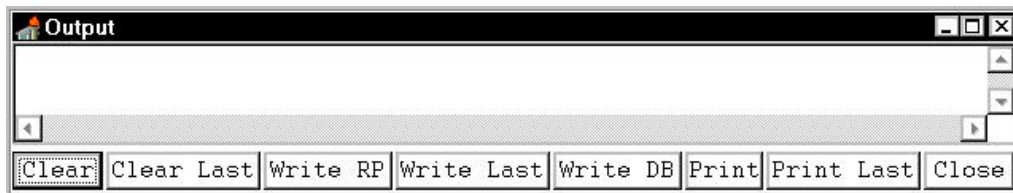
Figure 3.2.2 Toolbar buttons in the CMB8 Output window.

- – **Clear**: Erases all material currently printed in the Output window. The Output window cannot retain more than 32 Kbytes of information and must be periodically cleared during a CMB session.

- – **Clear Last:** Erases only the most recent output appearing in the Output window. This button may be repeatedly selected and the program will progress back through the output text blocks, clearing each in turn.

- – **Write RP:** Writes the entire contents of the Output window to the report output file (default CMBOUTRP.TXT).

- – **Write Last :** Writes the most recent addition to the Output window into the report output file. Write Last is used to record the final source contribution estimates for a sample along with the fitting species and source profile selections applied to obtain those contributions. It is also used to record the most recent information from other CMB commands that is displayed in the output window.

- – **Write DB:** Writes the results of the most recent fit to the data base output file (default CMBOUTDB.TXT). The data base format includes records of source contributions to each measured species for each sample.

3-4

- **Print:** Prints the entire contents of the display window using the current Windows 95 printer setting as defined by the Print Manager. Windows 95 also allows printer output to be directed to a file. For all three of the Write buttons the user is prompted for confirmation before an existing file is overwritten. The Courier 12 point font used in the Output display correctly aligns columns and is the default Windows 3.1 and HP LaserJet font.

- **Print Last:** Prints only the most recent addition to the Output window.

- **Close:** Closes the Output window.

- **Autofit (AUT, CTRL-A):** Autofit allows a single selection of fitting species and profiles to be applied to a selected list of samples without operator intervention. This feature is especially useful for model simulation testing and screening purposes. Autofit displays the Select Samples menu from which the desired samples are selected. It calculates source contribution estimates for each sample using the currently-selected fitting species, source profiles, and calculation options. After calculation, Autofit writes the results to the report and data base output files.

- **Present Source Contributions (SCN, CTRL-O):** This command presents a screen display of the fractional contribution of each source-type to each chemical species. These results are useful when contributions to species other than total mass are desired. This display also indicate which sources are the major and minor contributors to each chemical concentration.

- **Present Computed Averages (AVG, CTRL-L):** Averages and standard deviations of a series of source contribution estimates are calculated and displayed in the Output window. Only source contribution estimates written to the data base output file with the Write DB command are included in the average. The results of these averages can be written in the report output file with the Write Last command.

- **Present Source Profiles (PRO, CTRL-G):** Source profile entries (the mass fraction of each chemical component in each profile) are displayed in the Output window. This is useful to verify that input data files have been properly read and to identify the abundant components in each profile. The first row for each species displays the fractional abundance and the second row displays the standard deviation.

- **Present Receptor Concentrations (RCN, CTRL-R):** Ambient measurements for the current data record are displayed in the Output Window. This is useful to verify that input data files have been properly read in.

- **Present Normalized MPIN Matrix (MPN, CTRL-N):** The Modified Psuedo-Inverse Normalized matrix (MPIN) is displayed in the Output window for the fitting species. The MPIN identifies the influence of fitting species on the source contribution estimates.

- **Options (OPT, CTRL-T):** Several options and defaults have been added to CMB8 that are selected from the Options window, where various values and selections may be changed from their default values. Option settings are saved in a file named CMB8RSTR.DAT when the program is closed. This file is read when CMB8 is started for subsequent sessions and its contents dictate the new defaults.

Figure 3.2.3 CMB8 Options window.

– **Output File Format:** Sets the output file formats to blank delimited text (*.TXT), comma separated value (*.CSV), xBASE (*.DBF), or Lotus spreadsheet (*.WKS). Select the radio button that corresponds to the desired output format. The default setting is blank delimited text (*.TXT). xBASE programs such as dBASE and FoxPro specify that field names begin with an alphabetic character, and variable names for input files (source and species codes and mnemonics) must also begin with a letter rather than a number when the DBF format is for .

– **Display Dec's:** Sets the number of decimal places displayed in the output window and output files. This depends on the units used in the input data files. For example, data reported in ng/m^3 require fewer decimal places than values expressed in µg/m^3. This setting affects the "Show Fit" and "Write RP" display columns for inverse singular values, source contributions estimates, measured species concentrations, and calculated species concentrations. Click the edit box and type the desired number of decimal places. The default value is 5 and the maximum value is 6.

– **Max. Src. Unc. and Min. Src. Proj**.: These parameters allow the eligible space collinearity evaluation method of Henry (1992) to be implemented with each CMB calculation. The eligible space method uses: 1) maximum source uncertainty; and

3-6

2) minimum source projection on the eligible space. The maximum source uncertainty is expressed as a percentage of the total measured mass and is set to a default value of 20% in CMB8. The minimum source projection is set to a default value of 0.95. Maximum source uncertainty defines the eligible space as that spanned by eigenvectors with inverse singular values less than or equal to the maximum source uncertainty. Sources lying within the eligible space may be estimated with an uncertainty less than the maximum source uncertainty. This strict criteria of inclusion is relaxed somewhat and estimable sources are defined to be those with projections into the eligible space is at least the minimum source projection. Inestimable sources have small projections within the eligible space. Certain linear combinations of inestimable sources may be estimable, and the program lists these, if any exist. This may be understood as removing uncertainty by combining collinear sources. Different values for the maximum search uncertainty (ranging from 0 to 100%) and minimum source projections (ranging from 0 to 1.0) may be typed into the appropriate edit boxes and will be retained for subsequent source contribution calculations.

- **B and L:** Checking this box applies the Britt and Luecke (1973) linear least squares solution that is explained by Watson et al., 1984) when applied to CMB calculations. This option is available for research purposes and is not of utility in practical CMB applications. Checking the B and L box causes CMB8 to use the Britt and Luecke algorithm when performing the CMB fit.

- **S. Elim.:** Checking this box eliminates negative source contributions from the calculation. Fitting sources are eliminated one at a time, in sequential order, with fits performed after each elimination until all source contributions are positive.

- **Best Fit**: Checking this box cycles between the default fitting species and source profile combinations specified in the source and species selection input files until the best composite Fit Measure has been achieved. The first default fitting species selection is paired with the first default fitting sources selection, and so on. The fit with the largest Fit Measure is then displayed and becomes the current fit. After a Best Fit has been made the radio button in the default fitting species window and the radio button in the default fitting sources window are set to that used in the best fit.

- **Measure Weight:** These are the weights applied to each of the performance measures chi square, r-square, percent mass, and fraction of eligible sources (number in eligible space divided by number of fitting sources). Weights may be between 0 and 10,000 and are entered by typing into the appropriate edit boxes. Defaults are 1.0 for each performance measure.

- **RP Name:** Renames the default report file (CMBOUTRP.TXT) to any other name by typing into the edit box. If the file already exists, the user is asked for permission to overwrite the existing file with a new one.

- **DB Name:** Renames the default data base file (CMBOUTDB.TXT) to any other name by typing into the edit box. The file extension reflects the output format the edit box.

- **Units:** The units used in the Fit display may be changed by use of this edit box. The number of characters is limited to 5 or less.

- **Working Directory:** Output data files are written to the directory specified here. It defaults to the directory in which the CMB8 input files are located. To change this directory, edit the text in the edit box. This may be done at any time and results in a new working directory.

3.3 Graph

The graph menu, shown in Figure 3.3.1, allows visual outputs to be obtained for source profiles, ambient concentrations, and source contribution estimates.
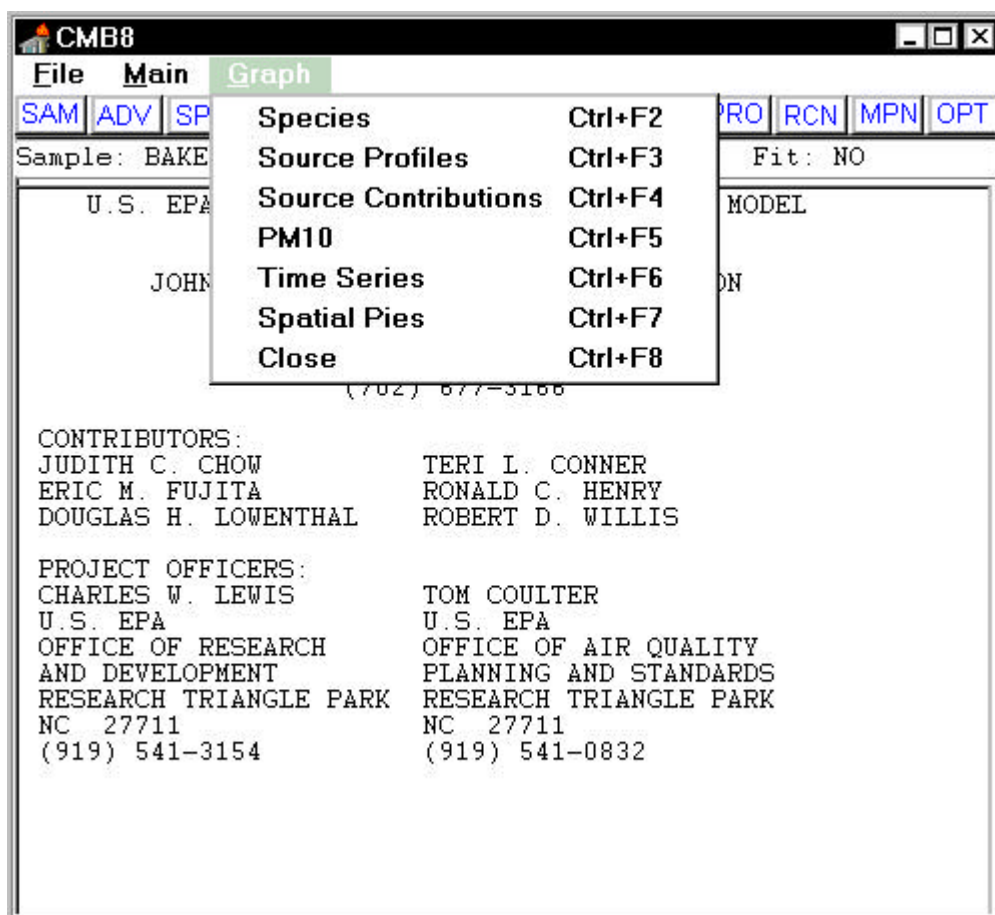
Figure 3.3.1. CMB8 Graph menu.

The Graph menu selections are:

- **Species (CTRL-F2):** Produces a bar graph of the species concentrations for the currently selected sample. The Y axis is a logarithmic scale, the height of the bar indicates the CMB8 calculated concentration, a horizontal line represents the measured concentration, and the error bars indicate the measurement precision. The graph adjusts to the size of the window, which can be re-sized by standard windows methods.

- **Source Profiles (CTRL-F3)**: A list box appears from which the desired profile can be selected. The Y axis is a logarithmic scale, the height of the bar indicates the abundance of each chemical species, and the error bars indicate the measurement precision. The graph adjusts to the size of the window, which can be re-sized by standard Windows methods.

- **Source Contributions (CTRL-F4):** Produces a pie chart of the source contributions for the current sample and the most recently calculated source contribution estimates.

- **PM10 (CTRL-F5):** Produces a pie chart of the source contributions for size TOTAL if the most recent two fits were to sizes FINE and COARS in any order.

- **Time Series (CTRL-F6):** - Creates a time series of stacked bars representing different source contributions. This selection operates calculations made by the most recent use of Autofit. Upon selection of this item the user is prompted for a site if more than one occurs among the Autofit sites. Similarly, the user is prompted for a size fraction if more than one occurs. A final prompt allows the user to reduce the number of fits displayed.

- **Spatial Pies (CTRL-F7)**: Plots pie charts of source contributions at specified site coordinates. This plot is useful for comparing source contributions among different sites as part of CMB model evaluation. It operates on source contribution estimates calculated by the most recent Autofit. Upon selection of this item the user is prompted for a date and start hour pair if more than one occurs among the Autofit calculations. Similarly, the user is prompted for a size fraction if more than one occurs. A final prompt allows the user to reduce the number of samples displayed. The remaining source contributions are then presented in a spatial series as pie charts using coordinates read from the ambient data selection file. The area of the pie charts is proportional to the total calculated mass, with the largest area being approximately 1 square inch on an 11" by 8.5" scale.

- **Close (CTRL-F8):** Closes the graphical output window.

The Graph window contains several command buttons, shown in Figure 3.3.2 that are used to record graphical outputs.

Figure 3.3.2 Toolbar buttons in the CMB8 Graph window.

– **Print:** Prints the current graph on the default printer.

– **Clip:** Copies the current graph to the clipboard. This allows graphs to be inserted into other documents such as Word for Windows documents by use of the insert command.

– **Orient:** Toggles the graph window orientation between landscape and portrait. An 8.5" by 11" aspect ratio is maintained.

Clear: Erases the graph in the Graph window.

– **Close:** Closes the graph window.

4. INPUT AND OUTPUT FILES

This section describes the structure of CMB8 input and output files and methods of generating these files. Each type of input file structure is illustrated with one of the test data sets packaged with CMB8.

4.1 File Naming Conventions

CMB input and output files can have any eight-character file name with a three-character extension that indicates the file type. The most convenient and universal naming convention is **PPXXXXYY.SSS**, where:

- **PP:** Type of file. Common definitions are:

  – **IN**-File identifying other input data file names.

  – **SO**-Source profile selection file, identifying default fitting profiles and source profile descriptions.

  – **PO**-Species selection file, identifying default fitting species.

  – **DS**-Data selection file, identifying samples to be selected from the ambient data file for apportionment during a CMB session.

  – **AD**-Ambient data file, containing the measured ambient concentrations and their precisions.

  – **PR**-Source profile file, containing mass-fraction chemical abundances and their uncertainties.

  – **OU**-Output file, containing report or data base output.

- **XXXX:** Study identifier. This four-letter code allows separate studies to be distinguished from one another.

- **YY:** Session or report identifier. This two-letter code can be assigned to variations on input data files or to distinguish report and data base output files. For example, input data files might be divided up by season or by sampling site to be evaluated in separate CMB modeling sessions. YY might take on the values 'WI' for winter, 'SP' for spring, 'SU' for summer, and 'FA' for fall. Default output filenames can be designated in the options menu with 'RP' identifying the report file and 'DB' representing the data base file. Output files should be written into separate directories, as designated in the Options menu, when different input files are used for the same project.

- **SSS:** File format identifier. The following file extensions are recognized by CMB8:

  – **IN8:** Input filename ASCII text file. CMB8 lists files with this extension when the program is executed and when CMB8 input files are requested using the File menu.

- **SEL:** Fitting profile, fitting species, and sample selection ASCII text files. CMB8 recognizes files with this extension has containing default selections that can be entered external to the program. This extension applies only to the SO, PO, and DS file types.

- **CSV:** Ambient data or source profile comma separated value ASCII text file. Each field is separated by a comma. Comma-delimited ASCII data base output files are written with this extension.

- **DBF:** X-base data base file generated by dBASE or FoxPro compatible data management software. Most commonly used spreadsheets offer this as an output option. DBASE or FoxPro output files are written with this extension.

- **TXT**: Ambient data or source profile data blank-delimited ASCII text file. Blank-delimited ASCII data base output files are written with this extension.

- **DAT**: Ambient or source profile data ASCII text file, blank delimited. File structure is identical to TXT extensions.

- **WKS:** Lotus 1-2-3 version 1 spreadsheet format. Most commonly used spreadsheets offer this as an output option. This is the most useful output format for the data base output file when source contribution estimates will be analyzed using a spreadsheet.

CMB8 converts the CSV, DBF, and WKS input data files to blank-delimited (TXT) files that are actually used by the program. This file carries the TXT suffix and may be used in subsequent modeling sessions to minimize startup time.

4.2   Input Files

Six data files are used for input to CMB8. Only the ambient and source profile data files are required, however. Though optional, the remaining four files provide substantial user convenience by establishing commonly used defaults and sample subsets that would otherwise need to be initialized each time CMB8 is run.

4.2.1   Input Filename File: INXXXXYY.IN8

This fixed format file contains a list of the names of other CMB8 input data files. This filename, which is normally entered in response to the first few prompts when CMB8 is started, consists of five lines as shown below. These lines, in succession, contain the names of the files which are described in the following sub-sections. INSJVF.IN8 is an example of this file structure used in CMB8.

```
1         2
01234567890
SOSJVF.SEL
POSJVF.SEL
DSSJVF.SEL
ADSJVF.CSV
PRSJVF.CSV
```

File name entries should be left justified. For the CMB8 32 bit version, the only restriction on file names is that they are acceptable to the operating system. This means that extended file names may be used. For the CMB8 16 bit version, each filename can be up to eight characters in length with up to a three-character suffix, and the fully qualified path plus file name should be less than 256 characters in length. The purpose of this file is to save the effort of keying in the input filename individually. If an INXXXXYY.IN8 filename is not entered at the appropriate prompt, CMB8 will request the names of individual data input filenames.

4.2.2 Source (SO*.SEL), Species (PO*.SEL), and Sample Selection (DS*.SEL) Input Files

The source, species and sample selection files provide defaults that do not have to be entered from the program each time a CMB8 session is begun. These files limit the profiles, species, and ambient data records to those listed in the selection files, even though a larger number may be included in the ambient and source profile data files. This means that the data files need not be edited when only subsets of variables are desired for a specific CMB8 modeling session. The source and species selection files also allow default sets of fitting profiles and species to be designated, making it unnecessary to select these at the beginning of each CMB8 session. Variable definitions can also be documented in these files. Sampling site coordinates can be documented in the sample selection file.

Following is an example of the source profile selection file SOSJVF.SEL:

```
0         1         2         3         4
12345678901234567890123456789012345678890
SJV001  SOIL01              *           STOCKTON AGRICULTURAL SOIL (PEAT)
SJV002  SOIL03          *               FRESNO PAVED ROAD
SJV003  SOIL04                          VISALIA AG SOIL (COTTON/WALNUT)
SJV004  SOIL05                          VISALIA AGRICULTURAL SOIL (RAISIN)
SJV005  SOIL06             *            VISALIA SAND AND GRAVEL
SJV006  SOIL07                          VISALIA URBAN UNPAVED
SJV007  SOIL08                          VISALIA PAVED ROAD
SJV008  SOIL09                          BAKERSFIELD AGRICULTURAL SOIL, ALKALINE
SJV009  SOIL10                          BAKERSFIELD AG SOIL, SANDY LOAM
SJV010  SOIL11                          BAKERSFIELD UNPAVED ROAD (OILDALE)
SJV011  SOIL12     *                    BAKERSFIELD PAVED ROAD
SJV012  SOIL13                          BAKERSFIELD WINDBLOWN URBAN UNPAVED
SJV013  SOIL14             *            BAKERSFIELD AG SOIL, WASCO SANDY LOAM
SJV014  SOIL15                          BAKERSFIELD AG SOIL, CAJON SANDY LOAM
SJV015  SOIL16                          BAKERSFIELD UNPAVED ROAD (RESIDENTIAL)
SJV016  SOIL17        *                 TAFT UNPAVED ROAD
SJV017  BAMAJC     * * * * *            BAKERSFIED CORDWOOD, MAJESTIC FIREPLACE
SJV018  MAMAJC                          MAMMOTH LAKES WOOD, MAJESTIC FIREPLACE
SJV019  MAFISC                          BAKERSFIELD WOOD, FISHER MAMA BEAR STOVE
SJV020  MADIEC                          MAMMOTH LAKES DIESEL TOUR BUSES (IDLING)
SJV021  BAAGBC                          BAKERSFIELD AG BURN (WHEAT AND BARLEY)
SJV022  ELAGBC                          EL CENTRO AGRI. BURN (WHEAT)
SJV023  FRCONC                          FRESNO HIGHWAY 40 CONSTRUCTION
SJV024  STAGBC                          STOCKTON AGRI. BURN (WHEAT)
SJV025  VIAGBC                          VISALIA AGRI BURN (WHEAT)
SJV026  VIDAIC                          VISALIA DAIRY/FEEDLOT DUST
SJV027  SFCRUC     * * * * *            SANTA FE CRUDE BOILER
SJV028  CHCRUC                          CHEVRON RACETRACK CRUDE BOILER
SJV029  MOTIBC                          MODESTO TIRE POWER PLANT
SJV030  SCRRFC                          STANISLAUS RESOURCE RECOVERY FACILITY
SJV031  CDCEMT                          NBS CEMENT DUST
SJV032  CDRKCR                          ROCK CRUSHING 1987 SCAB
```

```
SJV033   CDSAPL                              SANDBLASTING AND PLASTERING
SJV034   MARINE                              MARINE
SJV035   MOVES1                              MOVES-SS(NEA-E,WOB,T42,TVMT)
SJV036   MOVES2    * * * * *                 MOVES-SS(NEA-E,WOB,WOT,TVMT)
SJV038   MOVES3                              MOVES-SCAB(ARB-E,WOB,WOT,CM)
SJV039   MOVES4                              MOVES-SCAB(NEA-E,WOB,WOT,CM)
SJV040   MOVES5                              MOVES-SCAB(NEA-E,WB1,T42,CM)
SJV041   MPGYPU                              GYPSUM DUST, (TOTAL FROM CASO4)
SJV051   AMSUL     * * * * *                 AMMONIUM SULFATE
SJV052   AMBSUL                              AMMONIUM BISULFATE
SJV053   H2SO4                               SULFURIC ACID
SJV054   AMNIT     * * * * *                 AMMONIUM NITRATE
SJV055   HNO3                                NITRIC ACID
SJV056   NANO3       * * * *                 SODIUM NITRATE
SJV057   MVDEN1                              50% DIESEL, 20% LEADED, 30% UNLEADED
SJV058   MVDEN2                              75% DIESEL, 15% LEADED, 10% UNLEADED
SJV059   MVDEN3                              85% DIESEL, 10% LEADED,  5% UNLEADED
SJV060   OC                                  PURE ORGANIC CARBON
SJV061   LIME                                LIMESTONE
SJV062   SOIL28                              CROWS LANDING AGRI.
SJV063   SOIL29                              CROWS LANDING PAVED ROAD
SJV064   SOIL30                              KERN UNPAVED ROAD
SJV065   SOIL31                              KERN AGRI.
```

A source code with up to six characters is located in Columns 1 to 6 and an eight-character profile name is located in Columns 9 to 16. Asterisks in Column 19 designates the default fitting profiles when CMB8 is executed, and columns 21,23,25,27, 29, 31,33,35 and 37 can contain nine other default profile combinations that are selectable from the program. The maximum number of species is essentially unlimited. Text comments can be added to this file beginning at the 39th column to document the source profiles.

Following is an example of the species selection file POSJVF.SEL:

```
            1         2         3         4
12345678901234567890123456789012345678 90
  TMAC   TOT                                Mass by gravimetry (ug/m3)
  N3IC   NO3       * *     *                Nitrate by IC (ug/m3)
  S4IC   SO4       * *     *                Sulfate by IC (ug/m3)
  N4TC   NH4       * *     *                Ammonium by AC (ug/m3)
  KPAC   K-S       * *     *                Soluble Potassium by AA (ug/m3)
  NAAC   NA        * *     *                Soluble Sodium by AA (ug/m3)
  ECTC   EC        * *     *                Elemental Carbon by TOR (ug/m3)
  OCTC   OC        * *     *                Organic Carbon by TOR (ug/m3)
  ALXC   AL        * * * *                  Aluminum by XRF (ug/m3)
  SIXC   SI        * * * *                  Silicon by XRF (ug/m3)
  SUXC   S                                  Sulfur by XRF (ug/m3)
  CLXC   CL        * * * *                  Chloride by XRF (ug/m3)
  KPXC   K         * * * *                  Potassium by XRF (ug/m3)
  CAXC   CA        * * * *                  Calcium by XRF (ug/m3)
  TIXC   TI        * * * *                  Titanium by XRF (ug/m3)
  VAXC   V         * * * *                  Vanadium by XRF (ug/m3)
  CRXC   CR        * * * *                  Chromium by XRF (ug/m3)
  MNXC   MN        * * * *                  Manganese by XRF (ug/m3)
  FEXC   FE        * * * *                  Iron by XRF (ug/m3)
  NIXC   NI        * * * *                  Nickel by XRF (ug/m3)
  CUXC   CU          *                      Copper by XRF (ug/m3)
  ZNXC   ZN          *                      Zinc by XRF (ug/m3)
  BRXC   BR        *   * *                  Bromine by XRF (ug/m3)
  PBXC   PB        * * * *                  Lead by XRF (ug/m3)
```

A species code with up to six characters is located in Columns 1 to 6 and an eight-character species name is located in Columns 9 to 16. Asterisks in Column 19 designates the default fitting species when CMB8 is executed, and columns 21,23,25,27, 29, 31,33,35 and 37 can contain nine other default species combinations that are selectable from the program. The maximum number of species is essentially unlimited. Text comments can be added to this file beginning at the 39th column to document the meaning and units of the chemical components.

For the ambient data records selection file, columns 1 through 12 are for the site ID, columns 14 through 21 are for the date, columns 23 and 24 for the sample duration, columns 26 and 27 for the sample start hour, and columns 29-33 for the particle size fraction, if appropriate. Intermediate columns should be blank. An asterisk in column 35 selects a record. In addition columns 37 through 46 and columns 48 through 57 may contain x and y coordinates, respectively, for use in the Spatial Pie plots (see below). These should be in floating point format, e.g., 123.456, and should increase in value from left to right and from bottom to top. UTM coordinates are suitable as well as fractional longitudes and latitudes, if the longitudes are expressed as negative numbers.

Following is an example of the species selection file DSSJVF.SEL:

```
          1         2         3         4         5         6
1234567898012345678901234567890123456789012345678901234567890
BAKERS       02/27/89 24   0 FINE    * -119.01600 035.35800
CROWS        02/27/89 24   0 FINE    * -121.13000 037.37500
FELLOW       02/27/89 24   0 FINE    * -119.43900 035.13700
FRESNO       02/27/89 24   0 FINE    * -119.74000 036.70600
KERN         02/27/89 24   0 FINE    * -119.62500 035.59600
STOCKT       02/27/89 24   0 FINE    * -121.26700 037.95100
```

The file structure through the first 5 fields is that of the ambient data input, with columns 1-12 for the site name, columns 13-20 for the sample date, columns 22-23 for the sample duration (in hours), columns 25 and 26 for the sample start time (hour beginning), columns 28-32 for the particle size fraction, column 34 for an asterisk to identify this sample as a section for apportionment, columns 37-45 for the x-coordinate (west-east) of the corresponding sampling sites, and columns 47-55 for the y-coordinate (south-north) of the corresponding site. Site coordinates should be selected so that they are of increasing magnitude from west to east and from south to north. The negative longitude coordinate in columns 37 through 46 above meets that criterion. Coordinates should be in fractional units. UTM coordinates can also be used when they are all from the same zone. These coordinates are used for the spatial plotting display. Site coordinates are optional, and their columns are ignored if they are left blank. Only the first reference to a sampling site code requires coordinates to be supplied. These are assumed to be constant for all subsequent references to this site code.

4.2.3   Ambient Data Input File (AD*.CSV, AD*.DBF, AD*.TXT AD*.WKS)

Ambient data files may be formatted as column-separated values in ASCII text (CSV), xBASE (DBF), blank-delimited ASCII text (TXT), or Lotus Worksheet (WKS). The CSV and DBF formats are preferred, as they are easier to prepare in spreadsheet (e.g. Microsoft Excel, Corel QuatroPro, Lotus 123) and data base (e.g. Microsoft Access, dBASE) software than the

other formats. The WKS format creates large files and requires substantial translation time for CMB8 input and output, so it is the least desirable of these alternatives. The TXT format is most consistent with CMB7, so older CMB7 data files can be used for CMB8 input without modification. The appropriate file extension must be associated with each format, as CMB8 recognizes the file type by this extension.

Examples of each file type are provided with the CMB8DSJV.EXE test data. Following is an example of the ADSJVF.CSV file:

```
ID,DATE,DUR,STHOUR,SIZE,TMAC,TMAU,N3IC,N3IU,......,PBXC,PBXU
BAKERS,06/20/88,24,0,FINE,17.2788,0.9920,0.2816,0.1715,......,0.0236,0.0052
```

The delimited forms of this file do not require fixed format spacing, only that a comma (or a blank character for TXT files) separate each field from prior and subsequent fields. The first line contains the field identifiers, and these must be identical to those named in the selection files. The limitations on each field are:

Field 1:	Site ID (up to 12 characters)
Field 2:	Sampling date (up to 8 characters)
Field 3:	Sample duration (up to 2 characters)
Field 4:	Sample start hour (up to 2 characters)
Field 5:	Particle size fraction (up to 5 characters)
Field 6:	Mass concentration (any number of characters in integer, floating point, or exponential format)
Field 7:	Precision of mass concentration (same format as Field 6)
Field 8+2n:	Concentrations of chemical species (same format as Field 6), where n = 0, 1, 2, ...
Field 9+2n:	Precisions of species concentrations (same format as Field 6), where n = 0, 1, 2, ...

CMB8 always assumes that Field 6 is the total mass concentration, and it does not use this as a fitting species. For CMB8 he total number of ambient data records can reach into the thousands, limited only by computer memory. This makes it especially useful for examining multi-species hourly data obtained from automated gas chromatographs and time-of-flight mass spectrometers. For particles, up to four different size fraction identifiers may be used, and the user can select mnemonics that suit individual purposes. The size fraction names FINE and COARS are reserved for the $PM_{2.5}$ and coarse particle (PM_{10}-$PM_{2.5}$) size fractions that are most commonly measured in PM_{10} source assessment studies. When size fraction identifiers are used, an additional report is produced that sums the FINE and COARS source contribution estimates to provide the estimates for PM_{10}. Any other designator can be placed in the size column for non-segregated samples, such as "PM25" or "VOC". Where semi-volatile materials are being apportioned, the particle (PART) and gas (GAS) phases are good designations.

Missing values for chemical concentrations are designated by placing a -99. in the species concentration and precision fields. A species for which the value is missing cannot be used as a fitting species for that sample. Precisions that exceed zero must be assigned to all chemical concentrations used as fitting species. CMB8 will return an error message when it finds zero or negative precisions.

4.2.4   Source Profile Input File (PR*.CSV, PR*.DBF, PR*.TXT, PR*.WKS)

Source profile data files may be formatted as column-separated values in ASCII text (CSV), xBASE (DBF), blank-delimited ASCII text (TXT), or Lotus Worksheets (WKS). The CSV and DBF formats are the most portable and easily prepared. The appropriate file extension must be associated with each format, as CMB8 recognizes the file type by this extension. Examples of each file type are provided with the CMB8DSJV.EXE test data. Following is an example of the PRSJVF.CSV file:

```
PNO,SID,SIZE,N3IC,N3IU,......,PBXC,PBXU
SJV001,SOIL01,FINE,0.002700,0.004700,........,0.000000,0.000000
```

The delimited forms of this file do not require fixed format spacing, only that a comma (or a blank character for TXT files) separate each field from prior and subsequent fields. The first line contains the field identifiers, and these must be identical to those named in the selection files. The limitations on each field are:

Field 1:   Profile number or source code (up to six characters)
Field 2:   Source mnemonic (up to eight characters)
Field 3:   Particle size fraction (up to five characters)
Field 4+2n: Fraction of species in primary mass of source emissions (floating point or exponential format), where $n = 0, 1, 2, ...$
Field 5+2n: Variability of fraction of species in primary mass of source emissions (same format as Field 4), where $n = 0, 1, 2, ...$

The first record of the profile file contains the species codes for each field. These identifiers can be up to six alphanumeric characters in length, and must correspond to the identifiers used in the ambient data file. Source profile abundances are expressed in fractions of total mass, not in percent. This file does not contain a mass concentration field, as does the ambient data file, because all species abundances have been divided by this mass. The total number of records included depends on the number of species, number of sources, and size of the computer memory.

From one to four different size fraction identifiers may be used, but these must be the same as those used in the ambient data and sample selection files. Missing values for chemical species in source profile files can be replaced by a best estimate with a large uncertainty if they are to be used as fitting species, or with –99 if they will not be used. Default values of 0 for the fraction and 0.0001 to 0.01 for the precision are often chosen for species that are expected to be present in small abundances. This indicates that the species is present in source emissions at a concentration less than .01% to 1%. A smaller value may be appropriate for certain source-types and species. A precision value that exceeds zero <u>must</u> be entered for all fitting species. CMB8 will return an error message when it detects precisions that are less than or equal to zero.

4.3   Output Files

Report and data base output files are produced by CMB8.

4.3.1 Report Output File: RPXXXXRP.TXT

The report output file presents the source contribution estimates, standard errors, model performance measures, and measured and calculated chemical concentrations for each sample. The report written to the output file is identical to that which appears in the Output window during an interactive modeling session. It is in ASCII text format and can be imported into word processing programs to document the source contributions calculated for each sample. All information needed to independently repeat the source apportionment is contained in this report. Examples of the report are shown in Section 6.

4.3.2 Data Base Output File

The data base output file records the contribution of each source-type to each chemical species in a single data record. Sample identifiers and model performance measures are also included in each record. This file may be written in blank-delimited (TXT), comma separated values (CSV), xBASE (DBF), or Lotus 123 (WKS) formats (See Sec. 3). The file structure is:

Field 1:   Species Code
Field 2:   Species Name
Field 3:   Fitting flag; a '*' indicates a fitting species, while a '_' indicates a floating species
Field 4:   Sampling site identifier
Field 5:   Sampling date
Field 6:   Sample start hour
Field 7:   Sample duration
Field 8:   Particle size fraction
Field 9:   Measured species concentration
Field 10:   Precision of measured species concentration
Field 11:   R square value
Field 12:   Chi square value
Field 13:   Percent of measured mass
Field 14+2n: Source contribution estimate, $n = 0, 1, 2, ...$
Field 15+2n: Standard error of source contribution estimate, $n = 0, 1, 2, ...$

Fields 1, 2, and 4 through 10 record the sample information. Fields 3 and 11 through 13 provide information about the CMB calculation. The remaining fields correspond to each source profile in the PRXXXXYY file and contain the source contribution estimates and standard errors for these sources. A value of -99 is recorded when a profile was not used in the calculation.

The first record in this output file contains the field identifiers. All subsequent records contain data. Fields 14+2n and 15+2n are labeled with source codes and source contribution uncertainty columns are labeled with source names.

4.4   Creating Data Input Files

For blank delimited and comma separated value input files, there are three common methods of creating CMB8 input files: 1) manually entering the data in the correct format using a text editor or word processing program; 2) editing existing input files with a text editor or word processing program; or 3) transferring files from computerized data bases.

A text editor or word processor in text mode can be used to type entire input files. It is best to bring the example files into the editor, then insert the new values in the same locations as the existing values by using the editor in TYPEOVER mode. Spaces between fields should be entered with the space bar; tabs should <u>not</u> be set. Each line should be terminated with the ENTER key rather than using the wraparound feature present in many editors. No blank lines at the end of the file should be present. Completed files should be saved with an appropriate filename. The DOS EDIT command is a convenient and commonly available text editor, but it cannot read very long files. Notepad or Wordpad that are included as Windows accessories can also be used.

When data files have been prepared for other applications (e.g., source profiles may be common to several different data sets), these files may be cut and pasted to produce the needed input data files. Owing to differences in individual editing programs, the user is should consult the manual for the editing program to be used for directions on opening a copy of the existing file, deleting and adding material, saving the changes, and renaming the file. When word processors (e.g. Word or Wordperfect), the files must be saved as DOS text with line breaks, otherwise, extra information is included in the files that CMB8 cannot read.

Input files are most easily produced with spreadsheet or data base software. Many source profile and ambient data sets are available in data base management formats. Selections of data, field names, and data structure can be easily made by the data base software. These can be saved using the Save As or Export selections from the File menu. The CSV, DBF, and WKS formats can be selected from the "Save as type" option box that usually appears in the "Save As" window.

4.5 Reading Output Files

Report text files can be read directly into a word-processing program (e.g. Word or Wordperfect) where the detailed output for each sample can be usually be displayed on a single page with columns aligned using the Courier 8-point to 10-point font. A fixed-with font in which every character occupies the same space is needed for columns to be correctly aligned. Data base output files can be opened directly by data base or spreadsheet programs that recognize the CSV, DBF, TXT, and WKS extensions. The contents of the CMB8 output window can also be selected and copied to the clipboard for pasting into other Windows programs. Graphs made with CMB8 can be copied to the Windows clipboard with the Clip button, then pasted into a text box or frame in a word processing program.

5.   USING CMB8

This section illustrates CMB8 commands and operations using the San Joaquin Valley, CA, PM$_{2.5}$ data set. The other test data sets are provided as examples of additional data base file formats and for independent practice in CMB8 application and validation. These examples are most effective when accompanied by actual application of CMB8 on the user's computer.

5.1   Start CMB8

Start CMB8 by double-clicking on the CMB8 icon in the CMB80 folder, as shown in Figure 5.1.1, or by selecting it from the start menu. CMB8 may also be started from a DOS window by typing "CMB8" at the command line.
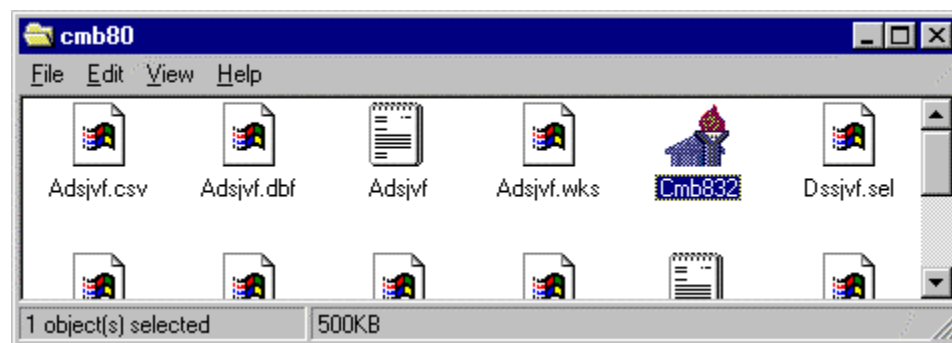
Figure 5.1.1. Double-click the CMB8.EXE icon to start.

When the "Restart from previous session?" box appears, click No. Clicking Yes will restore settings and data sets from the previous session. Try this option after completing this example.

5.2   Select Data Set

Click Yes when asked to use a CMB8 file names file. Clicking No will initiate a series of prompts for individual input file names. When the Open window appears, click on the INSJVF.IN8 selection. The default extension for file names files is IN8, and only files with this extension are listed in the selection box. To view all available files, replace *.IN8 with *.*, and all files in the CMB80 directory will appear in the selection box. The directory may be changed from the Look In box if files are located in another folder.

5.3   Examine the CMB8 Banner

Figure 5.3.1 shows the CMB8 banner. The parenthetical number in the second line after

CMB8 (97350) indicates the latest revision. It consists of the year (97) and julian day (350=12/22) on which CMB8 was most recently revised. It is good practice to verify this against the postings on U.S. EPA's bulletin board to assure that the most recent revision is being used. CMB8 is being continually improved as users respond with recommendations or difficulties. The data line underneath the toolbar shows the first ambient sample selected for CMB source apportionment, including its site, date, duration, start time, and size fraction. When the Fit indicator reads NO, it means that no calculations have yet been performed for this sample, and no source contribution estimates can be displayed. This line will always correspond to the current sample being analyzed.
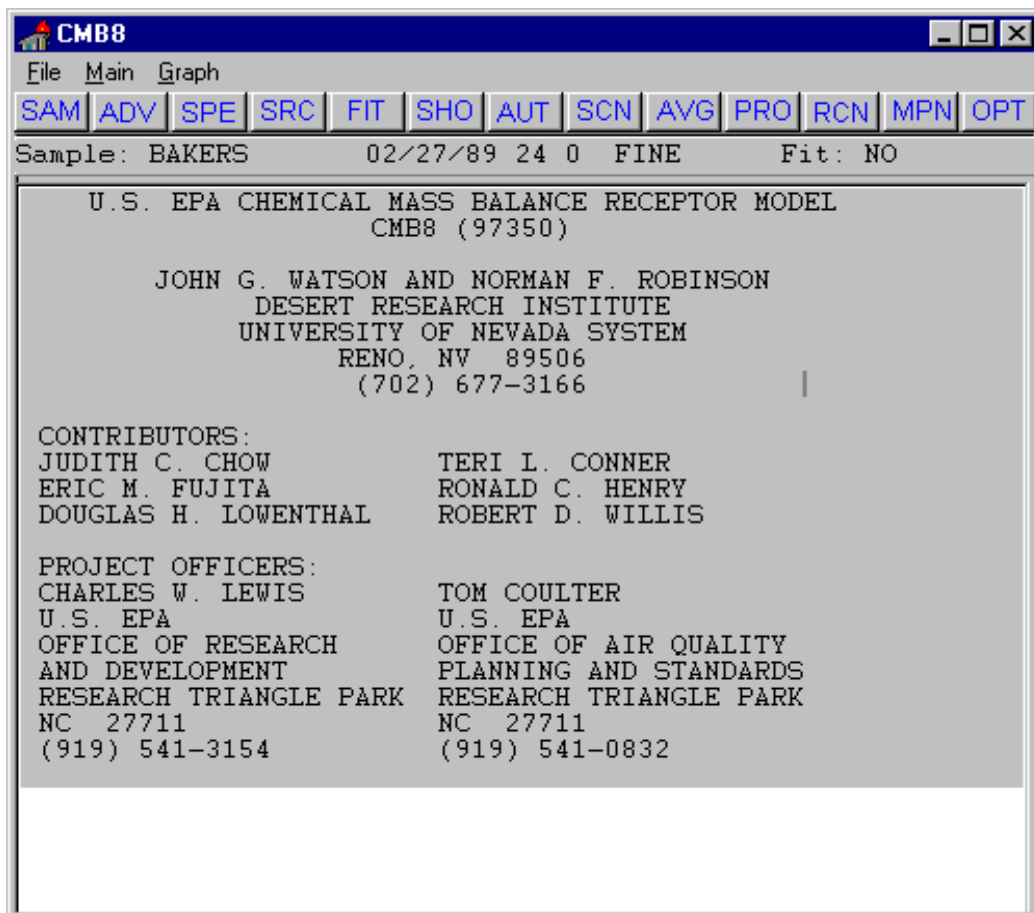
Figure 5.3.1. CMB8 banner page.

5.4   Set Options

Click on the OPT toolbar button (or select Options from the Main menu, or enter CTRL-T from the keyboard) to bring up the options window. Change the output file format to DBF by clicking the CMBOUTDB.DBF radio button. Change the RP Name to OUSJVFRP.TXT and the DB Name to OUSJVFDB.DBF by entering these over the default names. Change the Display Dec's value from 5 to 4, which is accommodates most $PM_{2.5}$ mass and chemical concentrations

expressed in $\mu g/m^3$. A value of 1 or 2 is best for concentrations expressed in ng/m^3 or for VOCs expressed in ppbC or $\mu g/m^3$. Leave the other options with their default values and click the OK button to record these options

Figure 5.4.1. Options window.

5.5   Select Samples

Click on the SAM toolbar button (or enter CTRL-M or click on Select Samples from the Main menu) to select the samples to be apportioned.
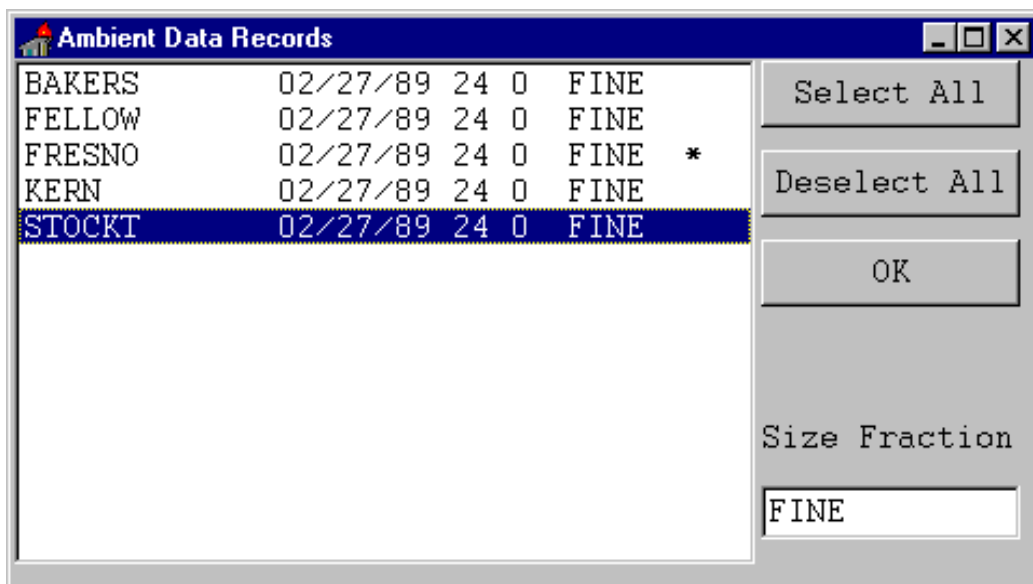
Figure 5.5.1. Sample selection window.

When this window appears, all five samples (specified in the sample selection input file) have asterisks to their right. Click on the top two and bottom two samples so that the asterisks disappear, leaving only the Fresno sample with an asterisk, as shown in Figure 5.5.1. Repeatedly clicking a sample causes the asterisk to appear (sample selected) or disappear (sample deselected). Clicking the Select All button places asterisks beside all samples in the list while clicking the Deselect All button removes them. Click the OK button to complete sample selection. At least one sample must be selected to quit this window and to continue with CMB8 operations.

5.6   Select Fitting Species and Profiles

Click the SPE and SRC buttons to bring up the Fitting Species and Fitting Sources windows. These windows can be moved to convenient positions on the desktop and resized using standard Windows techniques.
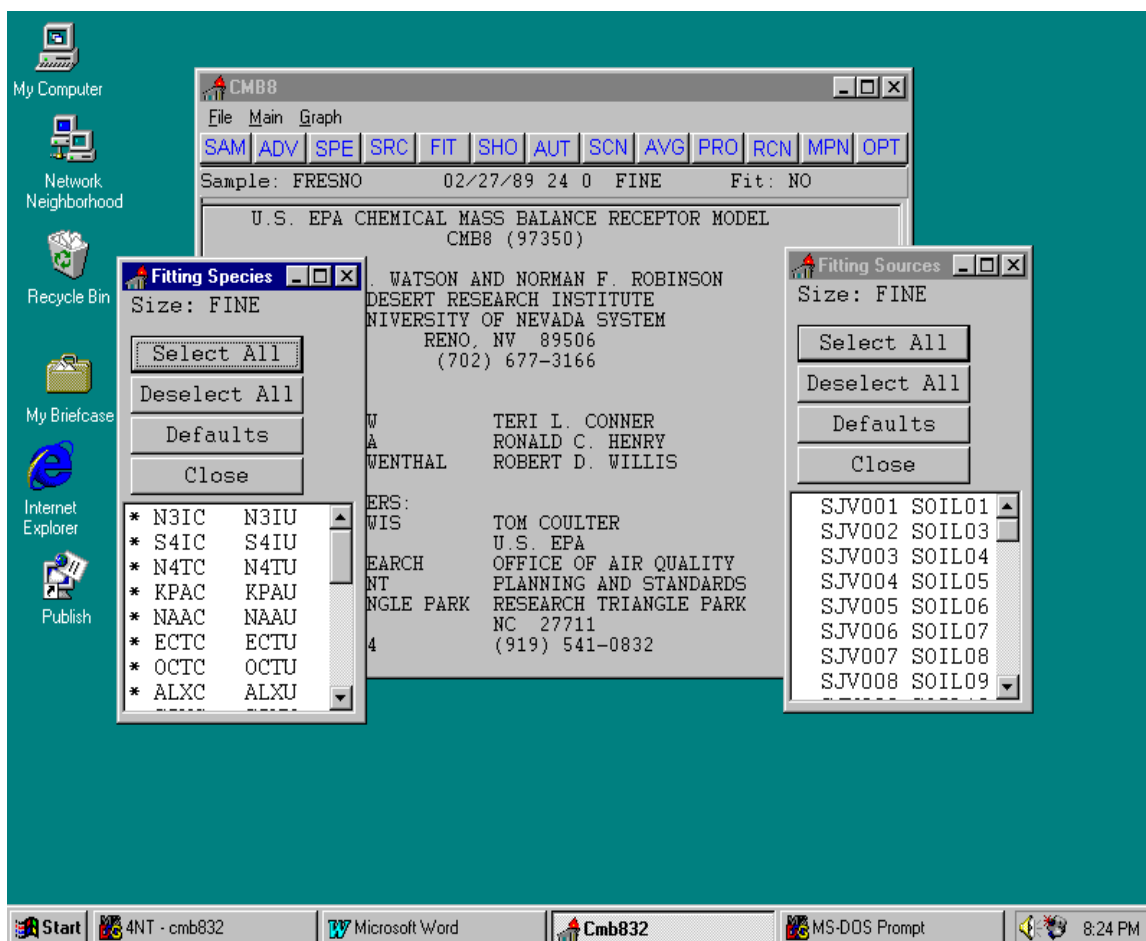
Figure 5.6.1. Fitting species and fitting source profile windows.

These windows remain open until the x-box in the upper right-hand corner is clicked. Windows can also be minimized using the standard windows techniques. They will return to their adjusted sizes and positions when the SPE and SRC buttons are pushed. An asterisk next to a species or profile mnemonic indicates that this is a fitting species or profile that will be used in the CMB calculation. Clicking on a mnemonic toggles between selection or deselection of the corresponding species or profile. The Select All and Deselect All buttons are used to place or remove an asterisk beside all mnemonics. The scroll bar to the right of each window is used to view the complete list of selections.

Clicking on the Defaults button in the Fitting Species window opens the Default Fitting Species window shown in Figure 5.6.2.
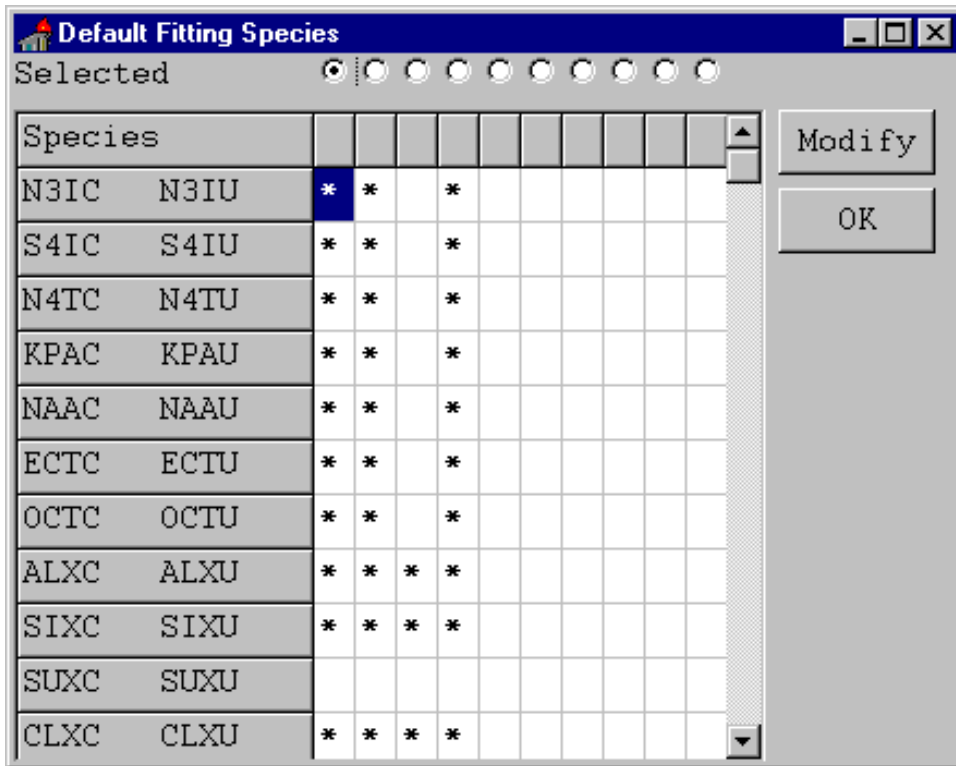
Figure 5.6.2. Default fitting species.

A similar window appears when the Defaults button is clicked in the Fitting Sources window. Up to ten combinations of fitting species and profiles can be defined in this window, with the first one being selected by default. The radio button at the top of the window indicates the combination that is currently in effect. The defaults indicated by asterisks in Figure 5.6.2 were defined in the species selection input file. They can be modified for the current CMB session by clicking the Modify button, then clicking in the appropriate box to toggle between selection and deselection. Only four combinations are illustrated in Figure 5.6.2, and six additional combinations may be entered into the blank columns to the right. These defaults combinations are convenient when CMB calculations are performed on samples from several locations or duringdifferent times of the year that have different contributors. They are also used by the Autofit option to iterate among different source combinations until the weighted Fit Measure is optimized. Click on OK to finalize the selection.

5.7   Perform CMB Calculation and Review Results

Click the FIT button and the output window displays the CMB output and performance measures. These are discussed in Section 6. In the fitting species window, select Defaults and click the third radio button that corresponds to a set of profiles more appropriate for Fresno in samples, click OK, then click the FIT button again. The source contribution report is illustrated in Figure 5.7.1. Scroll through the output to examine the most recent source contributions shown in Figure 5.7.1.

```
Output                                                              _ ☐ ✗
SOURCE CONTRIBUTION ESTIMATES -  SITE: FRESNO        DATE: 02/27/89  CMB8 (97350)
SAMPLE DURATION       24        START HOUR       0          SIZE:     FINE
      R SQUARE      .95    PERCENT MASS       82.4
   CHI SQUARE      1.40                DF       14
B and L: No    SRC ELIM: No
WEIGHTS:  CHISQR   1.000   R SQR   1.000  PCMASS   1.000  FRCEST    1.000


SOURCE
EST CODE    NAME     SCE(UG/M3)    STD ERR     TSTAT
----------------------------------------------------
YES SJV011 SOIL12      1.2050       .1568      7.6845
YES SJV017 BAMAJC      3.3775       .7551      4.4728
YES SJV027 SFCRUC       .2075       .1290      1.6081
YES SJV036 MOVES2      7.4446      1.8239      4.0816
YES SJV051 AMSUL       3.5468       .5563      6.3761
YES SJV054 AMNIT      25.7143      2.1241     12.1060
----------------------------------------------------


MEASURED CONCENTRATION FOR SIZE: FINE
      50.3+-      2.6

ELIGIBLE SPACE DIM. =   6 FOR MAX. UNC. =  10.0687  (20.% OF TOTAL MEAS. MASS)

1 / SINGULAR VALUE
----------------------------------------------------------------------------
   .1286     .1543     .5443     .7481    1.8285    2.1260
----------------------------------------------------------------------------


NUMBER ESTIMABLE SOURCES =   6 FOR MIN. PROJ. =   .95
 PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE
----------------------------------------------------------------------------

Clear│Clear Last│Write RP│Write Last│Write DB│Print│Print Last│Close
```

Figure 5.7.1. Output window with CMB source contribution estimates.

CMB outputs from both fits appear in the window, with the most recent output using the Fresno profile selection printed below the first apportionment with the default profiles. Click the Clear Last button and the most recent output disappears while retaining the previous output. Click the Clear button and all output displayed in the Output window disappears. Notice that the Fit indicator on the menu bar changed from NO to YES after the FIT button was clicked the first time.

Click the SHO button to recall the most recent calculation, then click the Write Last and Write DB buttons to record these results in the CMB8 output files. Experiment with the Print and Print Last buttons to obtain a hardcopy of calculation results from the Output window.

5.8   Examine Performance Measures

CMB performance diagnostics are described in Section 6. Most of these appear with the source contribution estimates in the Output window. The source contributions to species are obtained by clicking the SCN button to provide the output shown in Figure 5.8.1. This shows the fraction of each ambient chemical concentration contributed by each profile. In this example, it is apparent that the SOIL03 profile substantially overestimates aluminum and silicon concentrations.

Figure 5.8.1 also shows a convenient way to arrange the menu bar, the fitting species and profile windows, and the output window on the Windows desktop.

```
Output                                                          _ □ ×
SOURCE CONTRIBUTIONS (UG/M3) FOR SITE: FRESNO                     ▲
DATE: 02/27/89  DURATION: 24,  START HOUR: 0 ,  SIZE: FINE

                             CALC SPECIES(PER SOURCE)
              INDIVIDUAL RATIO = --------------------------
                             MEAS SPECIES(ALL SOURCES)
                              |
                                     SOURCE NAME
SPECIES SOIL12 BAMAJC SFCRUC MOVES2 AMSUL  AMNIT
  TMAU     .024   .067   .004   .148   .070   .511
  N3IU     .000   .001   .000   .008   .000  1.035
  S4IU     .005   .017   .015   .080   .896   .000
  N4TU     .000   .000   .000   .000   .137   .823
  KPAU     .042   .901   .001   .000   .000   .000
  NAAU     .052   .024   .008   .000   .000   .000
  ECTU     .004   .118   .000   .886   .000   .000
  OCTU     .038   .251   .000   .618   .000   .000
  ALXU    1.374   .000   .000   .089   .000   .000
  SIXU    1.250   .000   .000   .381   .000   .000
  SUXU     .006   .016   .010   .070   .786   .000
  CLXU     .068  1.006   .001   .034   .000   .000
  KPXU     .139   .795   .000   .004   .000   .000
  CAXU    1.245   .053   .003   .119   .000   .000
  TIXU    9.439   .000   .035   .124   .000   .000
  VAXU     .226   .000  1.064   .047   .000   .000
  CRXU     .181   .000   .010   .000   .000   .000           ▼
◄                                                            ►
Clear Clear Last Write RP Write Last Write DB Print Print Last
```

Figure 5.8.1. Source contributions to species performance diagnostic.

Clicking on the MPN button displays the Modified Psuedo Inverse (MPIN) matrix in the output window. This matrix shows which species have the largest influence on the source contribution estimates from each profile. Examining these weights suggests sensitivity tests to determine the extent to which source contributions vary with changes in profile abundances or the selection of fitting species.

```
Output                                                                    _ □ X

TRANSPOSE OF SENSITIVITY MATRIX FOR SITE: FRESNO
DATE: 02/27/89  DURATION: 24,  START HOUR: 0 ,  SIZE: FINE

                                    SOURCE NAME
   SPECIES SOIL12 BAMAJC SFCRUC MOVES2 AMSUL  AMNIT

    N3IU    -.01    .00    .01    .04   -.11   1.00
    S4IU     .00    .00    .00    .01   1.00   -.19
    N4TU     .01    .00   -.01   -.04    .12    .89
    KPAU    -.03    .49    .00   -.07    .00    .00
    NAAU     .02    .01    .01   -.01    .00    .00

 Clear  Clear Last  Write RP  Write Last  Write DB  Print  Print Last  Close
```

Figure 5.8.2. MPIN matrix in the Output window.

These displays can be written to the report profile by clicking on the Write Last or Write RP buttons, or they can sent to the printer with the Print or Print Last buttons.

5.9   Autofit

The Autofit option calculates source contributions for all selected samples without having to examine each one. Click on the AUT button, then click on Yes in the confirmation box. When the sample selection box appears, click on Select All, then on the OK button. Watch the status line below the CMB8 toolbar change as the source contribution estimates are calculated for each of the selected samples. Data are written to the RP and DB output files as part of the Autofit procedure so that they can be examined later.

5.10   Examine Source Profiles and Receptor Concentrations

Click on the PRO button and all source profile chemical abundances are listed in the Output window, as shown in Figure 5.10.1. This is a good way to verify that data have been correctly read from the input files and to determine which species are most abundant in each profile. The top number in each species row contains the fractional mass abundance and the second row contains the uncertainty of that abundance.

```
Output                                                    _ □ ×

SOURCE PROFILES FOR SIZE FINE

                       SOIL01    SOIL03    SOIL04    SOIL05    SOIL06

TMAC    TMAU          1.0000    1.0000    1.0000    1.0000    1.0000
                       .0000     .0000     .0000     .0000     .0000
N3IC    N3IU           .0027     .0000     .0000     .0003     .0000
                       .0047     .0036     .0030     .0026     .0658
S4IC    S4IU           .0004     .0050     .0000     .0000     .0000
                       .0013     .0066     .0011     .0009     .0238
N4TC    N4TU           .0006     .0003     .0000     .0000     .0000

Clear  Clear Last  Write RP  Write Last  Write DB  Print  Print Last
```

Figure 5.10.1. Source profile listing.

Clicking on the RCN button writes the receptor concentrations for the current sample to the Output window. This display can also be used to verify input data.

5.11   Graph Source Profiles, Ambient Concentrations, and Source Contributions

Select Species from the Graph menu, and a display similar to Figure 5.11.1 appears. The height of the bar shows the calculated concentration, the horizontal line shows the measured concentration, and the error bar shows the precision of the receptor measurements.
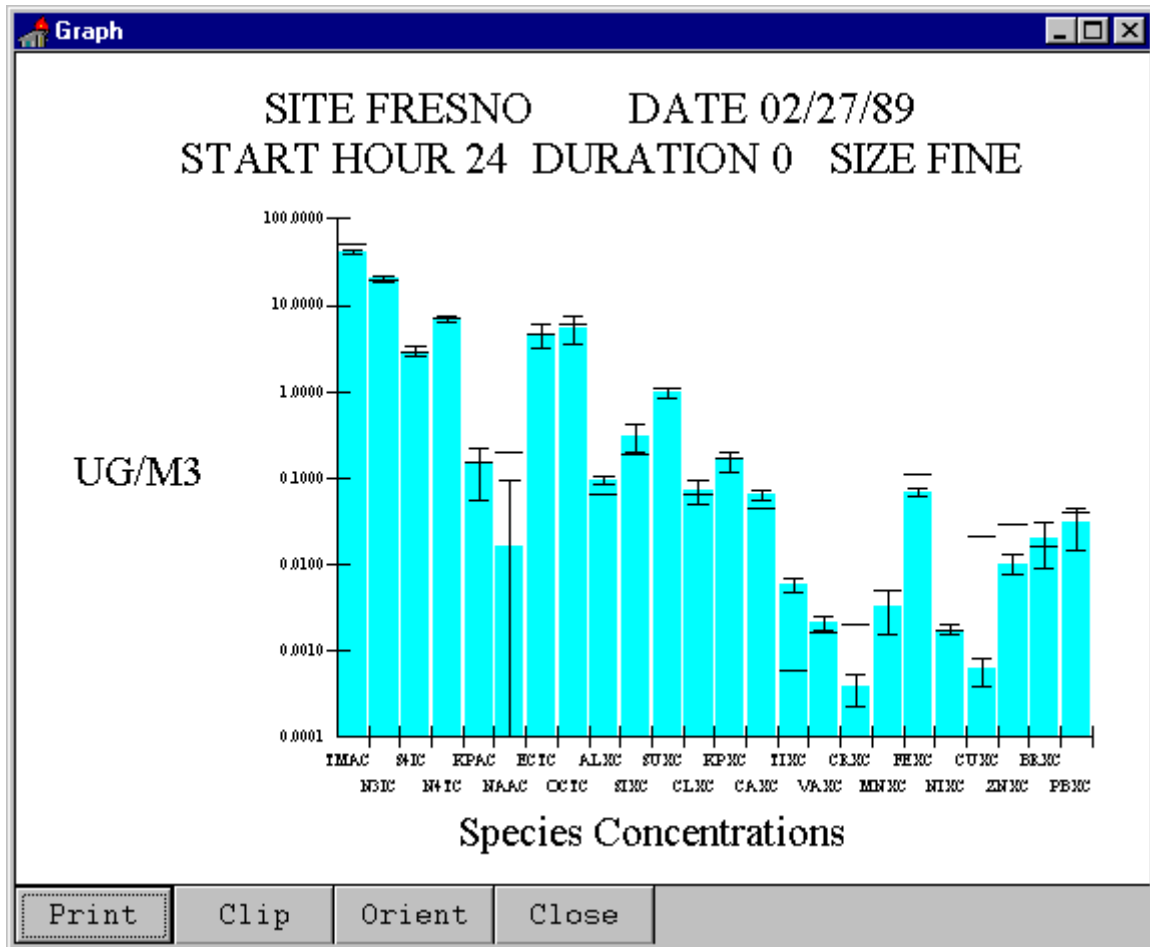
Figure 5.11.1. Example of Species selection from the Graph menu.

Try the same for the Source Profiles option in the Graph menu. In this case a selection box appears from which the desired source may be marked by clicking on its mnemonic, then graphed when the OK button is clicked. Click on the Source Contributions option in the Graph menu to create a pie plot of source contributions for the current sample. Experiment with the Clip, Print, and Orient buttons as described in Section 3. In particular, Clip one of the graphs and paste it into another Windows program such as Microsoft Word.

5.12   Plot Spatial Pies

After Autofit has been executed and source contribution estimates are available for all sites, select the Spatial Pies option from the Graph menu. Click the OK button when asked to select sites. Sites are selected by depressing the CTRL key while clicking on the desired sites. Click the OK button to create a spatial display similar to that of Figure 5.12.1.

5.13   Exit CMB8

From the Files menu, click the Exit button to close CMB8.
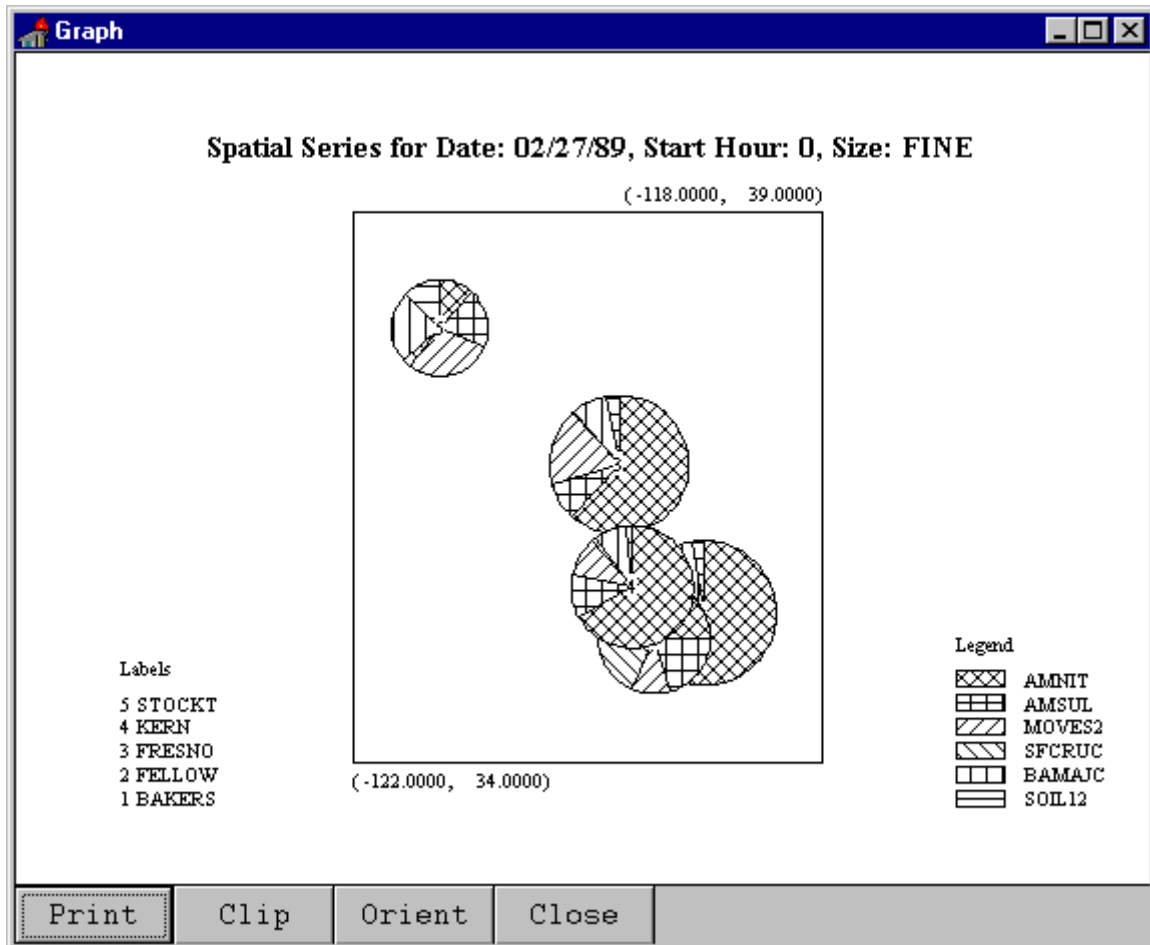
Figure 5.13.1. Example of a spatial pie plot of CMB source contributions.

5.14   Working with Large Amounts of Data

Open the INSJVF.IN8 file in a text editor (e.g. DOS edit or Windows Notepad), replace the third line containing DSSJVF.SEL with XXXXX, and save the modified file as INSJVF1.IN8. Start CMB8 and select Yes to restart from previous session. Open the INSJVF1.IN8 input file from the File menu. This preserves previously selected options and window placement.

Examine the Ambient Data Records window with the SAM button. All available samples in the data input file are now available for examinations. Select all of the samples and perform Autofit. If a window such as that illustrated in Figure 5.14.1 appears, the source contributions for that sample have not converged after 20 iterations. Select Continue with iteration delta=20 several times to determine whether or not convergence can be achieved with a few more

iterations. The maximum number of iterations can be changed in the options menu by selecting Continue. Change iteration delta. If no convergence can be achieved, there is probably excessive collinearity for this sample that must be treated individually. Note the sampling site, date, and time, then select Exit without viewing results to continue with Autofit.

To plot a time series of source contributions, select Time Series from the Graph menu, select one of the sites from the site list menu that appears, and click OK. Select the dates to be plotted from the sample menu that appears by scrolling or clicking with the mouse while depressing the CTRL key. No more than 25 samples may be selected for an individual time series plot. Click OK, and a stacked bar plot similar to that in Figure 5.14.2 results.
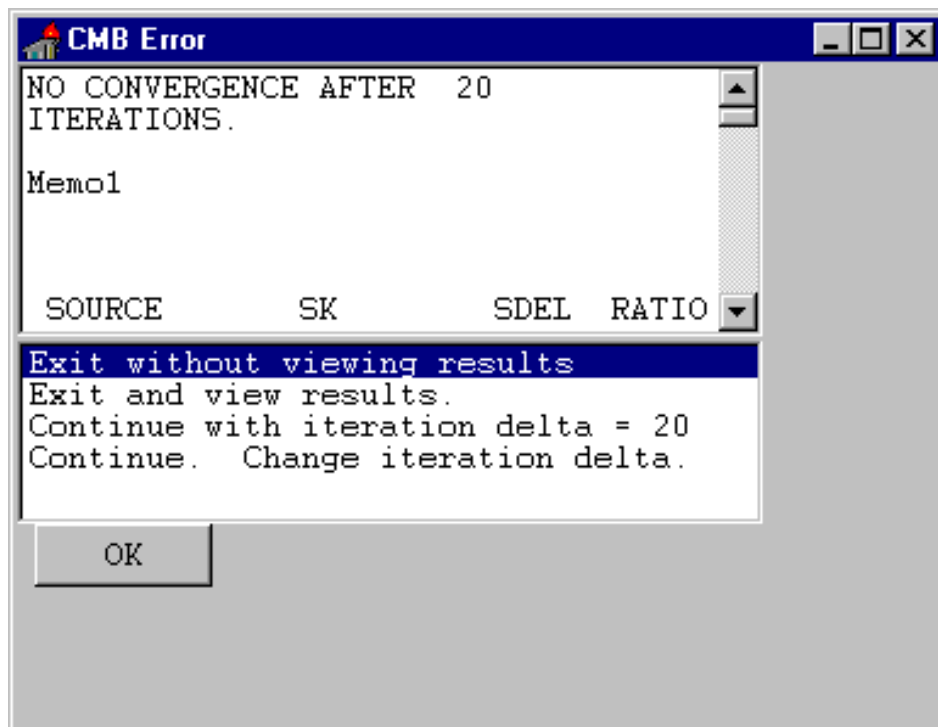
Figure 5.14.1. Options that appear when a CMB calculation does not converge.
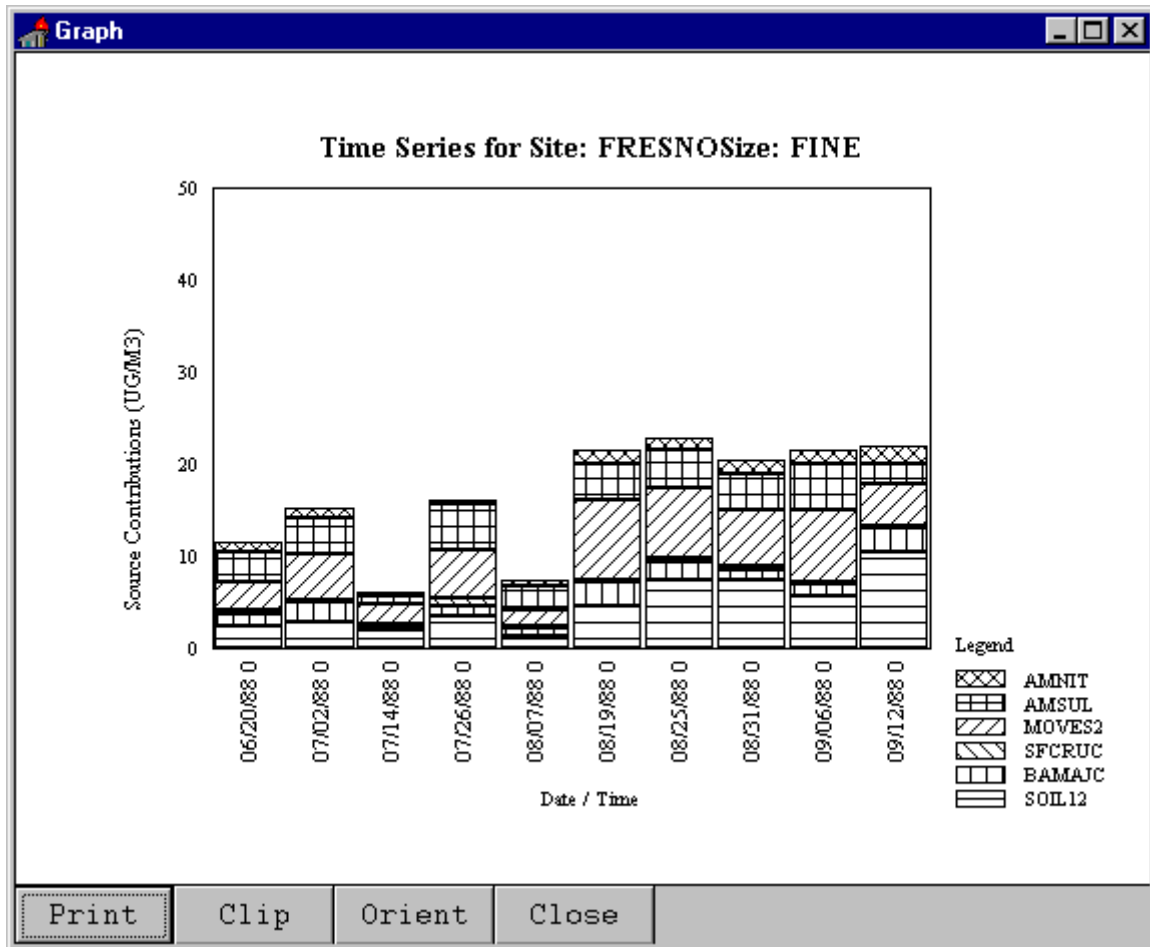
Figure 5.14.2. Example of stacked bar chart output.

Exit CMB8 and start a word processing program such as Microsoft Word. Open the OUSJVF1RP.TXT file and experiment with different font types and sizes to produce a summary of CMB output reports for review.

Start a spreadsheet program such as Microsoft Excel. In the File/Open selection, navigate to the CMB80 directory and select OUSJVFDB.DBF. Figure 5.14.3 shows an example of the data base output imported into a spreadsheet.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	
1	ELCOD	ELNAME	I	SITEID	DATE	ST	DR	SIZE	CONC	UCONC	RSQUAR	CHISQUAR	PCMASS	SJV001	SOIL01	SJV
2	TMAC	TMAU		BAKERS	02/27/89	0	24	FINE	53.5523	2.7206	0.9330	2.2606	89.3275	-99.0000	0.0000	-9
3	N3IC	N3IU	*	BAKERS	02/27/89	0	24	FINE	18.0102	0.9166	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
4	S4IC	S4IU	*	BAKERS	02/27/89	0	24	FINE	3.9818	0.2138	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
5	N4TC	N4TU	*	BAKERS	02/27/89	0	24	FINE	7.6140	0.3902	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
6	KPAC	KPAU	*	BAKERS	02/27/89	0	24	FINE	0.1022	0.0219	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
7	NAAC	NAAU	*	BAKERS	02/27/89	0	24	FINE	0.0981	0.0536	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
8	ECTC	ECTU	*	BAKERS	02/27/89	0	24	FINE	4.7498	0.5854	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
9	OCTC	OCTU	*	BAKERS	02/27/89	0	24	FINE	6.4803	0.8302	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
10	ALXC	ALXU	*	BAKERS	02/27/89	0	24	FINE	0.0494	0.0237	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
11	SIXC	SIXU	*	BAKERS	02/27/89	0	24	FINE	0.1244	0.0390	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
12	SUXC	SUXU	_	BAKERS	02/27/89	0	24	FINE	1.8470	0.0936	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
13	CLXC	CLXU	*	BAKERS	02/27/89	0	24	FINE	0.0740	0.0082	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
14	KPXC	KPXU	*	BAKERS	02/27/89	0	24	FINE	0.1274	0.0089	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
15	CAXC	CAXU	*	BAKERS	02/27/89	0	24	FINE	0.0686	0.0074	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
16	TIXC	TIXU	*	BAKERS	02/27/89	0	24	FINE	0.0040	0.0184	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
17	VAXC	VAXU	*	BAKERS	02/27/89	0	24	FINE	0.0155	0.0031	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
18	CRXC	CRXU	*	BAKERS	02/27/89	0	24	FINE	0.0005	0.0026	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
19	MNXC	MNXU	*	BAKERS	02/27/89	0	24	FINE	0.0052	0.0009	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
20	FEXC	FEXU	*	BAKERS	02/27/89	0	24	FINE	0.1110	0.0126	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
21	NIXC	NIXU	*	BAKERS	02/27/89	0	24	FINE	0.0217	0.0015	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
22	CUXC	CUXU	_	BAKERS	02/27/89	0	24	FINE	0.0187	0.0663	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
23	ZNXC	ZNXU	_	BAKERS	02/27/89	0	24	FINE	0.0556	0.0395	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
24	BRXC	BRXU	*	BAKERS	02/27/89	0	24	FINE	0.0129	0.0009	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9
25	PBXC	PBXU	*	BAKERS	02/27/89	0	24	FINE	0.1406	0.0089	0.9330	2.2606	89.3275	-99.0000	-99.0000	-9

Figure 5.14.3. Example of CMB8 output imported into a spreadsheet.

The output file contains the contribution of each source to each measured species in each sample. Fitting species are identified by an asterisk in the third column, and performance measures follow. Source contribution estimates and their standard errors are presented in subsequent columns, identified by mnemonics in the first row. Contributions from non-fitting profiles for a sample are identified as –99. Common spreadsheet data analysis tools can be used to select records for different chemical species, to group contributions from different profiles representing the same source type, calculating average contributions, and plotting results.

6.   CMB PERFORMANCE MEASURES

This section describes the different performance measures that are used to evaluate the validity of source contribution estimates. Greater detail on the use of the performance measures is presented by Watson et al. (1998). The performance measures are presented in three separate displays when the Calculate Source Contributions or Show Fit menu options are invoked: 1) the source contribution display; 2) the eligible space display; and 3) the species concentration display. Each of these displays is discussed below.

6.1   Source Contribution Estimates Display

An example of a source contribution table display is shown below:

```
SOURCE CONTRIBUTION ESTIMATES -  SITE: FRESNO      DATE: 02/27/89  CMB8 (97350)
SAMPLE DURATION          24       START HOUR         0           SIZE:    FINE
      R SQUARE          .96    PERCENT MASS       83.2
    CHI SQUARE         1.06                  DF        13
B and L: No    SRC ELIM: No
WEIGHTS:  CHISQR   1.000   R SQR   1.000  PCMASS   1.000  FRCEST   1.000


SOURCE
EST CODE    NAME      SCE(UG/M3)     STD ERR      TSTAT
----------------------------------------------------
YES SJV002 SOIL03       1.2276        .1588       7.7281
YES SJV017 BAMAJC       3.4511        .7703       4.4800
YES SJV027 SFCRUC        .2043        .1290       1.5834
YES SJV036 MOVES2       7.3898       1.8264       4.0461
YES SJV051 AMSUL        3.5726        .5566       6.4184
YES SJV054 AMNIT       25.3561       2.1106      12.0137
YES SJV056 NANO3         .6795        .3511       1.9354
----------------------------------------------------


MEASURED CONCENTRATION FOR SIZE: FINE
     50.3+-      2.6
```

Source contribution estimates are the main output of the CMB model. The sum of these concentrations approximates the total mass concentration. Negative source contribution estimates are not physically meaningful, but they can occur when a source profile is collinear with another profile or when the source contribution is close to zero. Collinearity is usually identified in the eligible sources display. When the absolute value of a positive or negative source contribution estimate is less than its standard error, the source contribution is undetectable. Two or three times the standard error may be taken as an upper limit of the source contribution in this case.

The standard errors reflect the precisions of the ambient data, the source profiles, and the amount of collinearity among different profiles. Standard errors should be reported with every source contribution estimate. The standard error is a single standard deviation. There is about a 66% probability that the true source contribution is within one standard error and about a 95% probability that the true contribution is within two standard errors of the source contribution estimate.

The T-statistic (TSTAT) is the ratio of the source contribution estimate to the standard error. A TSTAT value less than 2.0 indicates that the source contribution estimate is at or below

a detection limit. Low TSTAT values for several source contributions may be caused by collinearities among their profiles; this will be indicated by the Similarity/Uncertainty Clusters.

The reduced chi square, degrees of freedom, R square, percent mass, and fit measure are performance measures for the least squares calculation.

The chi-square is the weighted sum of squares of the differences between the calculated and measured fitting species concentrations. The weighting is inversely proportional to the squares of the precisions in the source profiles and ambient data for each species. Ideally, there would be no difference between calculated and measured species concentrations and chi-square would equal zero. A value less than 1 indicates a very good fit to the data, while values between 1 and 2 are acceptable. Chi-square values greater than 4 indicate that one or more species concentrations are not well explained by the source contribution estimates. The degrees of freedom equal the number of fitting species minus the number of fitting sources. The degrees of freedom is needed when statistical significance tests are applied to the chi-square value.

The R-square is the fraction of the variance in the measured concentrations that is explained by the variance in the calculated species concentrations. It is determined by a linear regression of measured versus model-calculated values for the fitting species. R-square ranges from 0 to 1.0. The closer the value is to 1.0, the better the source contribution estimates explain the measured concentrations. When R-square is less than 0.8, the source contribution estimates do not explain the observations very well with the fitting source profiles and/or species.

Percent mass is the percent ratio of the sum of the model-calculated source contribution estimates to the measured mass concentration. This ratio should equal 100%, although values ranging from 80 to 120% are acceptable. If the measured mass is very low (< 5 to 10 $\mu g/m^3$), percent mass may be outside of this range because the precision of the mass measurement is on the order of 1 to 2 $\mu g/m^3$.

The Fit Measure is calculated using the algorithm

Fit_measure = Wt_chisqr * (2 / chisqr)

         + Wt_R-square *R-square

         + Wt_pcmass * pcmass / 100 (for pcmass < 100) or + Wt_pcmass * 100 / pcmass
           (for pcmass > 100)

         + Wt_fracest * Frac_Est

where chisqr, rsquare, and pcmass are the performance measures for reduced chi-square, R-square, and per cent mass, respectively, and where Frac_Est is the ratio of the number of estimable fitting sources to the total number of fitting sources. The weights accorded to each of these variables (Wt_chisqr, Wt_R-square, Wt_pcmass , and Wt_fracest) are set to 1.0 by default. These weights may be changed in the Options window.

The BANDL flag indicates whether or not the Britt and Luecke (1973) solution was used - N for no, Y for yes. The SRC ELEM flag indicates whether or not the fit was obtained using source elimination. The number of decimal places used in presenting the individual source data is 5. This is the default value, but it may be changed in the Options menu .

6.2   Eligible Space Display

The eligible space display identifies the potential for collinearity and the potential reductions in standard errors in the source contribution estimates when source profiles are combined. An example appears below for the PACS1, 8/13/77, COARS test data set.

```
ELIGIBLE SPACE DIM. =   7 FOR MAX. UNC. =  10.0687  (20.% OF TOTAL MEAS. MASS)

1 / SINGULAR VALUE
-------------------------------------------------------------------------------
   .1285     .1562     .3497     .5445     .7625    1.8313    2.1128
-------------------------------------------------------------------------------


NUMBER ESTIMABLE SOURCES =   7 FOR MIN. PROJ. =   .95
PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE    PROJ. SOURCE
-------------------------------------------------------------------------------
1.0000 SJV002  1.0000 SJV017  1.0000 SJV027  1.0000 SJV036  1.0000 SJV051
1.0000 SJV054  1.0000 SJV056
-------------------------------------------------------------------------------


ESTIMABLE LINEAR COMBINATIONS OF INESTIMABLE SOURCES
OEFF. SOURCE   COEFF. SOURCE   COEFF. SOURCE   COEFF. SOURCE    SCE         STD ERR
-------------------------------------------------------------------------------
-------------------------------------------------------------------------------
```

Henry's (1992) eligible space treatment uses uses the maximum source uncertainty, expressed as a percentage of the total measured mass, and the minimum source projection. These may be changed from their default values of 20% and 0.95, respectively, in the Options menu. The maximum source uncertainty defines a space, called the eligible space, to be that spanned by those eigenvectors with inverse singular values less than or equal to the maximum source uncertainty. The first part of this display gives the eligible space dimension and the uncertainty used in its calculation. This is followed by the inverse singular values.   Source profiles lying within the eligible space may be estimated with an uncertainty less than the maximum source uncertainty. This strict criteria of inclusion is relaxed somewhat and estimable sources are defined to be those with projections into the eligible space of more than the specified minimum source projection.

The next part of the display gives the number of estimable sources, the minimum source projection used in the calculation, and the projections of each profile vector into the estimable space. These inestimable sources are caused by excessive similarity (collinearity) among the source profiles or by high uncertainties in the individual source profiles. The standard errors associated with the source contribution estimates of one or more inestimable sources are usually very large, often too large to allow an adequate separation of these source contributions to be made.   Inestimable sources will not appear if the two above-stated criteria are not met. This absence of inestimable sources means that the source contributions can be resolved in the specific application. Since ambient data uncertainties, and relative levels of source contributions vary from sample to sample, it is possible that a given set of profiles may appear in the inestimable space for one set of ambient data, but not for another set. For this reason, it is impossible to

decide <u>a priori</u> that a set of profiles is collinear or not. The decision must be made for each set of data and each set of profiles combined with those data.

If collinearity is the cause of these excessive standard errors, then certain linear combinations of inestimable sources may be estimable, and the final part of the display lists these, if any exist. This may be understood as removing uncertainty by combining collinear sources. This linear combination may be more useful than the individual source contribution estimates if the standard error of the linear combination is substantially lower than the standard errors of each source contribution estimate. The treatment does not allow differentiation among the contribution estimates of the sources contained in the linear combination, however. For a more complete treatment of this topic see [[[App.]]]]. Also, as above for the individual source data, the number of decimal places used in the presentation of the inverse singular values is that set in the Options menu.

6.3   Species Concentration Display

An example of the species concentration display is shown below:

```
SPECIES CONCENTRATIONS -  SITE: FRESNO        DATE: 02/27/89       CMB 8.0
SAMPLE DURATION      24        START HOUR         0          SIZE:    FINE
      R SQUARE       .96   PERCENT MASS        83.2
    CHI SQUARE      1.06              DF          13

SPECIES-------I---MEAS-----------------CALC------------RATIO C/M----RATIO R/U
TMAC   TMAU        50.3433+-  2.5652  41.8809+-  2.7727    .83+-   .07     -2.2
N3IC   N3IU    *   19.2608+-   .9793  20.3104+-  1.9713   1.05+-   .12      .5
S4IC   S4IU    *    2.8779+-   .1653   2.9238+-   .3694   1.02+-   .14      .1
N4TC   N4TU    *    7.0496+-   .3636   6.6966+-   .5847    .95+-   .10     -.5
KPAC   KPAU    *     .1496+-   .0235    .1419+-   .0854    .95+-   .59     -.1
NAAC   NAAU    *     .1982+-   .0566    .1929+-   .0762    .97+-   .47     -.1
ECTC   ECTU    *    4.5527+-   .5979   4.5762+-  1.4756   1.01+-   .35      .0
OCTC   OCTU    *    5.9985+-   .8449   5.4261+-  1.8067    .90+-   .33     -.3
ALXC   ALXU    *     .0641+-   .0242    .1189+-   .0135   1.85+-   .73     2.0
SIXC   SIXU    *     .1869+-   .0392    .3353+-   .1071   1.79+-   .69     1.3
SUXC   SUXU        1.0952+-   .0565    .9798+-   .1232    .89+-   .12     -.9
CLXC   CLXU    *     .0641+-   .0080    .0704+-   .0221   1.10+-   .37      .3
KPXC   KPXU    *     .1695+-   .0107    .1624+-   .0429    .96+-   .26     -.2
CAXC   CAXU    *     .0450+-   .0071    .0484+-   .0077   1.07+-   .24      .3
TIXC   TIXU    *     .0006<    .0193    .0065<    .0010  10.80< *****      .3
VAXC   VAXU    *     .0016<    .0081    .0021<    .0004   1.32<   6.70      .1
CRXC   CRXU    *     .0020+-   .0017    .0004+-   .0002    .19+-   .18     -.9
MNXC   MNXU    *     .0049+-   .0009    .0036+-   .0018    .73+-   .39     -.7
FEXC   FEXU    *     .1125+-   .0129    .0759+-   .0086    .67+-   .11     -2.4
NIXC   NIXU    *     .0017+-   .0010    .0017+-   .0002   1.02+-   .62      .0
CUXC   CUXU         .0214<    .0679    .0006<    .0002    .03<    .09     -.3
ZNXC   ZNXU         .0295<    .0403    .0105<    .0025    .36<    .49     -.5
BRXC   BRXU    *     .0166+-   .0010    .0200+-   .0112   1.20+-   .68      .3
PBXC   PBXU    *     .0399+-   .0056    .0320+-   .0153    .80+-   .40     -.5
```

This display shows how well the individual ambient concentrations are reproduced by the source contribution estimates. This display offers clues concerning which sources might be missing or which ones do not belong in the calculation. Fitting species are marked with an asterisk in the column labeled 'I'.

The column labeled RATIO R/U contains the ratio of the signed difference between the calculated and measured concentrations (the residual) divided by the uncertainty of that residual (square root of the sum of the squares of the uncertainty in the calculated and measured concentrations). The R/U ratio specifies the number of

6-4

uncertainty intervals by which the calculated and measured concentrations differ. When the absolute value of the R/U ratio exceeds 2, the residual is significant. If it is positive, then one or more of the profiles is contributing too much to that species. If it is negative, then there is an insufficient contribution to that species and a source may be missing. The sum of the squared R/U for fitting species divided by the degrees of freedom yields the chi square. The highest R/U values for fitting species are the cause of high chi square values. Also, as above for the individual source data, the number of decimal places used in the presentation of the species data is that set in the Options menu.

6.4 Additional Performance Measures

Main menu choice Present Source Contributions produces a table that shows the fraction of each species' calculated ambient concentration contributed by each source in the fit. The sources that are major contributors to each species can be determined by examining this display. An example of this display is shown below:

```
SOURCE CONTRIBUTIONS (UG/M3) FOR SITE: FRESNO
DATE: 02/27/89  DURATION: 24,  START HOUR: 0 ,  SIZE: FINE

                                CALC SPECIES(PER SOURCE)
             INDIVIDUAL RATIO = ------------------------
                                MEAS SPECIES(ALL SOURCES)
                                     SOURCE NAME
SPECIES SOIL03 BAMAJC SFCRUC MOVES2 AMSUL  AMNIT  NANO3
 TMAU     .024   .069   .004   .147   .071   .504   .013
 N3IU     .000   .001   .000   .008   .000  1.020   .026
 S4IU     .002   .017   .014   .080   .902   .000   .000
 N4TU     .000   .000   .000   .000   .138   .811   .000
 KPAU     .027   .920   .001   .000   .000   .000   .000
 NAAU     .014   .024   .008   .000   .000   .000   .927
 ECTU     .006   .120   .000   .879   .000   .000   .000
 OCTU     .034   .257   .000   .614   .000   .000   .000
 ALXU    1.766   .000   .000   .089   .000   .000   .000
 SIXU    1.415   .000   .000   .378   .000   .000   .000
 SUXU     .006   .016   .010   .070   .792   .000   .000
 CLXU     .036  1.028   .001   .033   .000   .000   .000
 KPXU     .142   .812   .000   .003   .000   .000   .000
 CAXU     .900   .054   .003   .118   .000   .000   .000
 TIXU   10.639   .000   .034   .123   .000   .000   .000
 VAXU     .230   .000  1.047   .046   .000   .000   .000
 CRXU     .184   .000   .010   .000   .000   .000   .000
 MNXU     .301   .000   .004   .422   .000   .000   .000
 FEXU     .670   .000   .004   .001   .000   .000   .000
 NIXU     .072   .000   .949   .000   .000   .000   .000
 CUXU     .011   .000   .000   .017   .000   .000   .000
 ZNXU     .100   .105   .018   .133   .000   .000   .000
 BRXU     .007   .021   .000  1.175   .000   .000   .000
 PBXU     .111   .000   .000   .691   .000   .000   .000
```

Another diagnostic is the transpose of the normalized modified pseudo-inverse matrix (MPIN). This matrix indicates the degree of influence each species concentration has on the contribution and standard of error of the corresponding source category. MPIN is normalized such that it takes on values from -1 to 1. Species with MPIN absolute values of 1 to 0.5 are associated with influential species. Noninfluential species have MPIN absolute values of 0.3 or less. Species with absolute values between 0.3 and 0.5 are ambiguous but should generally be considered noninfluential.

An example display of this diagnostic is shown below:

```
TRANSPOSE OF SENSITIVITY MATRIX FOR SITE: FRESNO
DATE: 02/27/89  DURATION: 24,  START HOUR: 0 ,  SIZE: FINE

                                  SOURCE NAME
  SPECIES SOIL03 BAMAJC SFCRUC MOVES2 AMSUL  AMNIT  NANO3
    N3IU   -.01    .00    .01    .04   -.11   1.00    .05
    S4IU    .00    .00    .00    .01   1.00   -.20    .01
    N4TU    .01    .00   -.01   -.04    .12    .90   -.06
    KPAU   -.02    .50    .00   -.08    .00    .00    .00
    NAAU    .00    .00    .00    .00    .01   -.12   1.00
    ECTU   -.17   -.01    .00   1.00   -.08    .01    .00
    OCTU   -.11    .16    .00    .71   -.06    .01    .00
    ALXU    .83   -.06   -.02   -.06    .01    .00    .00
    SIXU    .43   -.06   -.01    .17   -.01    .00    .00
    CLXU   -.05    .90    .00   -.10   -.01    .00   -.01
    KPXU    .04   1.00    .00   -.17    .00    .00   -.01
    CAXU    .76    .01   -.01    .06   -.01    .00    .00
    TIXU    .07    .00    .00   -.01    .00    .00    .00
    VAXU    .00    .00    .13    .00   -.01    .00    .00
    CRXU    .04    .00    .01   -.01    .00    .00    .00
    MNXU    .08   -.06    .00    .39   -.03    .00    .00
    FEXU   1.00   -.06    .00   -.17    .01    .00    .00
    NIXU   -.02    .00   1.00    .00   -.06    .01   -.01
    BRXU   -.11   -.07    .00    .70   -.06    .00    .00
    PBXU   -.05   -.08    .00    .68   -.06    .00    .00
```

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