



RECEPTOR MODEL TECHNICAL SERIES

VOLUME III

User's Manual For Chemical Mass Balance Model

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By

Hugh J. Williamson
Dennis A. DuBose

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EPA Project Officer: Warren P. Freas

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77 West Jackson Boulevard, 12th Floor
Chicago, IL 60604-3580

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PREFACE

Receptor Model Technical Series Volume III User's Manual for Chemical Mass Balance Model

Recent improvements in air sampling and analytical techniques have stimulated rapid growth in new techniques of source impact analysis using receptor models. These models "decode" the chemical fingerprints and variability of the ambient aerosol to back-calculate source impacts. Unlike source (dispersion) models that estimate source impacts from emission rate, meteorology and stack parameters, receptor techniques estimate source contributions to the total, fine, coarse, or inhalable particulate mass using data from ambient aerosol measurements.

This document is the third of a series describing how receptor models can be used by State and local regulatory agencies to identify particulate source impacts. Volume I (EPA-450/4-81-016a) provides an overview of Receptor Model Applications, while Volume II (EPA-450/81-016b) focuses on the Chemical Mass Balance (CMB) technique, model theory and input requirements.

This report documents an interactive FORTRAN computer program which performs aerosol source apportionment through weighted least squares with options to include effective variance and ridge regression features. The original version of the program, which performed weighted least squares with the effective variance option, was developed at the Oregon Graduate Center based on the Doctoral Dissertation of Dr. John Watson. The program was later modified at Oregon by Dave Torkelson. The current version has been developed under contract to EPA by Drs. Hugh Williamson and Dennis DuBose of Radian Corporation. In the latest version, the ridge regression feature was added, along with various modifications intended to enhance the ease of use of the program.

The computer program described in this manual is available on magnetic tape as EPA-450/4-83-014b and can be acquired in either of two ways:

1. Government and nonprofit agencies may obtain a copy of the program by sending a blank magnetic tape and written request to:

Chief, Technology Development Section
Air Management Technology Branch/MDAD (MD-14)
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711
Attention: Receptor Model Request

2. Others wishing a copy of the program may purchase it from the National Technical Information Service, Springfield, Virginia 22161, telephone (703) 557-4650.

This report has been reviewed by the Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, and approved for publication as received from Radian Corporation. Approval does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

ABSTRACT

This report presents a discussion of aerosol source apportionment. Chemical mass balance (CMB) equations are used to estimate the contributions of the important source types to an ambient particulate concentration. Separate analyses are ordinarily performed for the fine and coarse size fractions. The basic solution technique discussed is weighted regression analysis. In this method, the more accurate ambient concentration data are weighted more heavily to produce a better solution. The analysis technique can be modified to include the effective variance feature, the ridge regression feature, or both. In the effective variance feature, the uncertainties of all input data (ambient and source) are employed in the analysis. Effective variance calculations produce a weighted least squares solution with refined estimates of the weights. The ridge feature is especially designed to handle cases in which the particulate emissions from different sources are chemically similar. Ridge regression potentially allows more resolution in the source apportionment, in that a more complex set of sources can often be handled. The report also documents an interactive computer program which performs source apportionment using the techniques discussed above. A set of examples of CMB applications is presented to illustrate the various options of the program.

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SECTION 1

MODEL OVERVIEW

1.1 Background and Purpose

This report documents an interactive computer program which can be used to perform an analysis of the sources of ambient aerosol concentrations. Figure 1-1 summarizes the objectives to be achieved by source apportionment. The problem to be addressed consists of the presence of objectionable or hazardous atmospheric particulate matter. Source apportionment provides an approach for addressing the problem.

"Source apportionment," "source receptor modeling," and "chemical mass balance (CMB) analysis" are terms which refer to a statistical analysis through which the major contributors to ambient aerosol pollution are identified. Specifically, an ambient particulate concentration is apportioned among its sources. For example, if the concentration was $110 \mu\text{g}/\text{m}^3$, the analysis might indicate that $40 \mu\text{g}/\text{m}^3$ came from source A, $35 \mu\text{g}/\text{m}^3$ from source B, etc. The "sources" are source categories such as windblown dust, automobiles, petroleum refineries, etc. The exact set of sources which should be included varies geographically. Separate source apportionments are usually performed for the fine and coarse size fractions. Apportionment can be made based on the concentrations determined from a single aerosol sample or based on the average concentrations from a set of samples.

The required chemical inputs consist of (1) the chemical characteristics of the aerosols from each source type to be considered, and (2) the chemical characteristics of the ambient aerosols. It is also possible to use the uncertainties of the input data in the analysis. This allows the more accurate data to be weighted more heavily to produce a better solution.

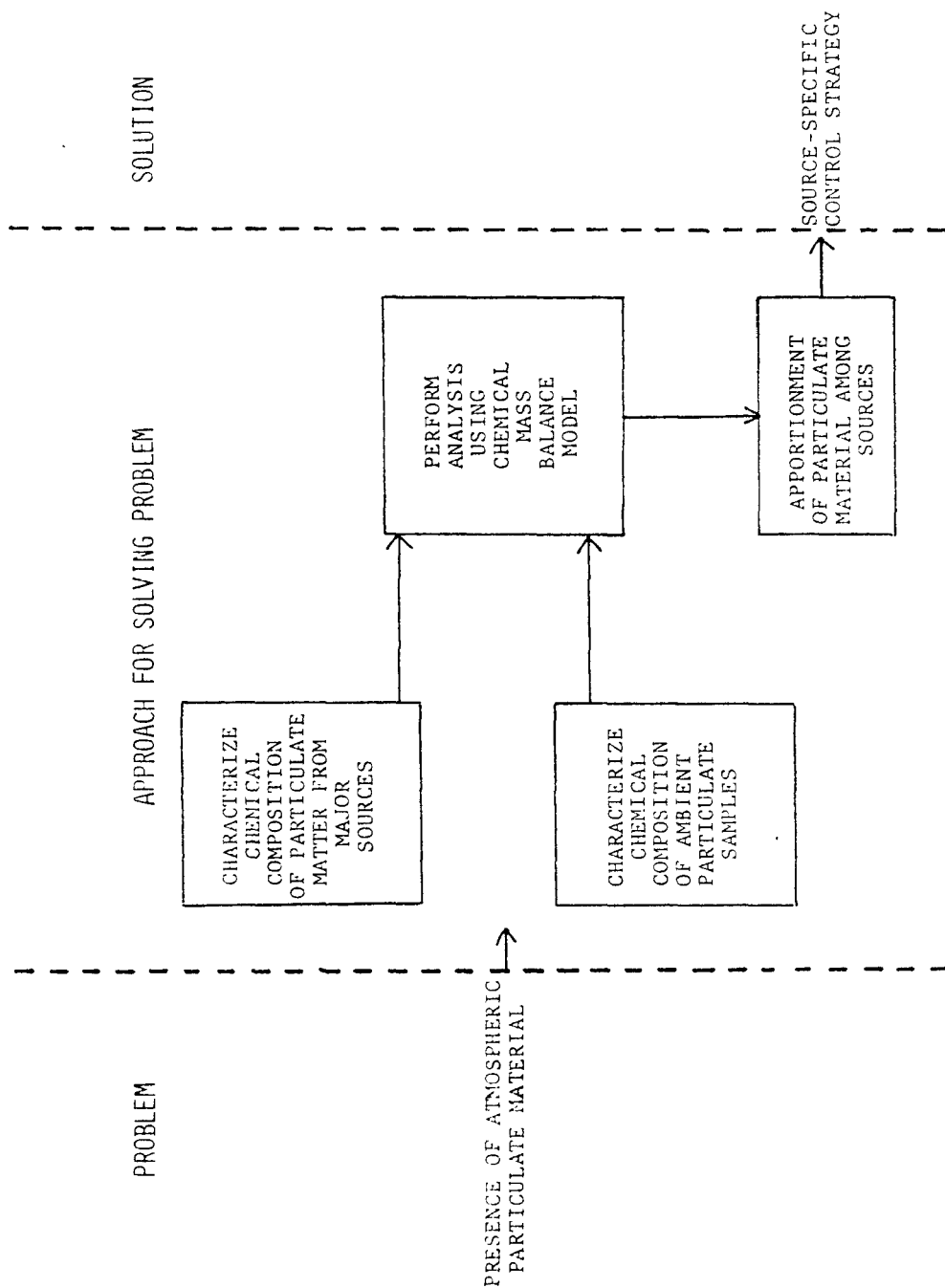


Figure 1-1. Source Apportionment of Ambient Particulate Material

A statistical model which employs a set of mass balance equations is used to apportion the particulate matter among its sources. A separate mass balance equation is employed for each of a set of chemical species. An additional mass balance equation employs the aerosol concentration for the size fraction being considered. The inputs (1) and (2), above, contain information regarding the set of species selected for inclusion in the analysis and for the aerosol concentration.

The knowledge of which sources are the largest contributors to the ambient aerosols plays an important role in the formulation of a source-specific control strategy. Additionally, source apportionment is a valuable research tool.

The basic solution technique discussed herein is weighted least squares. In this technique, the more accurate input ambient concentrations are weighted more heavily to produce a better solution. The following major options regarding the solution technique are also available:

- (1) Effective variance calculations--a procedure through which the errors in the complete set of chemical input data are taken into account in weighting the more accurate data more heavily to produce a better solution. If effective variances are not used, the uncertainties in only the ambient concentration data are used.
- (2) Ridge regression--a feature designed specifically to handle cases in which the aerosols of two or more sources are chemically similar. Soil, road dust, and asphalt production is ordinarily such a set. If conventional statistical techniques are used rather than ridge regression, it is usually necessary to combine sources with similar aerosols into groups and apportion the ambient aerosols among the groups. The separate contributions of the different sources within a group, however, are not quantified. Ridge regression provides an opportunity to achieve greater resolution through analysis of a larger set of separate source categories.

Even with ridge regression, however, it is not possible to separate the influences of sources whose aerosols are chemically indistinguishable. A discussion of the pros and cons of ridge regression is presented in Section 2.2.

1.2 Definitions of Terms

This subsection presents a set of definitions of technical terms used in this report. The reader may wish to scan the definitions for an introduction to the terms and to refer to them while reading the report. Expanded discussions of many of the terms as they apply to source apportionment are presented in the following sections.

Source receptor analysis--a type of statistical analysis through which an ambient aerosol concentration is apportioned among its sources. The terms "source apportionment analysis" and "chemical mass balance (CMB) analysis" are used in the same sense in this report.

Chemical mass balance equation--an equation in which a mass or concentration is equated to the sum of its parts. In this context, the ambient aerosol concentration is equated to the aerosol concentration due to source one plus the concentration due to source two, etc. Similar mass balance equations are used for individual chemical species which make up the ambient aerosol.

Vector--a one-dimensional array of numbers, e.g., $X_1, X_2, \dots, X_i \dots X_n$.

Matrix--a two-dimensional array of numbers, e.g., X_{ij} , $i=1$ to n , $j=1$ to m . Notice that a given row or column of a matrix can be thought of as a vector.

Source signature--a quantification of the chemical characteristics of the aerosols from a particular source. A source signature is a vector

whose i^{th} value is the fraction of the aerosol from a specific source which is composed of chemical species i . Suppose, for example, that the soil in an area consisted of 20% silicon. Then the entry in the source signature for soil corresponding to silicon would be 0.20.

Source signature matrix--a matrix whose columns are the signatures for a set of sources.

Standard error--the standard deviation of the error in a quantity. For example, the standard errors of the ambient concentrations and of the source signatures are required inputs if a CMB analysis is performed using weighted least squares with effective variances.

Error variance--the square of a standard error.

Regression analysis--a statistical method by which a mathematical model is developed to predict a dependent variable in terms of one or more other variables. The coefficients in the model are selected so as to minimize the sum of squares of the differences between the observed and predicted values in the data set being used. Regression is also referred to as ordinary least squares.

Regression coefficient--a parameter in a regression model whose value is estimated from the data.

Weighted least squares--the same as regression analysis, except that the values of the dependent variable are weighted according to their uncertainties in order to produce a more accurate solution.

Effective variance--the error variance in an equation, taking into account the uncertainties in both the dependent variable and the predictor variables. In a refinement of weighted least squares, effective variances are used in place of the error variances of the dependent variable alone.

The objective is to weight the data according to all input uncertainties in performing the model development.

Observation--the vector of values of all variables being considered in an analysis for one case. In regression analysis, for example, an observation consists of a value of the dependent variable and the corresponding values of the independent, or predictor, variables.

Sample size--the number of observations used in a statistical analysis.

Iterative solution--an approximate answer to a particular problem accomplished by computing a succession of estimates of the true answer. If the procedure is successful, the estimates approach the true answer as the number of approximations generated increases. Thus, beyond some point, consecutive estimates differ very little from each other. As is discussed in Section 2, an iterative solution is required if effective variances are used.

Iteration--the set of calculations required to produce one of the estimates in an iterative procedure.

Correlation coefficient (R)--a measure of the strength of the linear relationship between two variables. If the correlation is one, a perfect linear relationship exists, and one variable increases as the other increases. If the correlation is minus one, a perfect linear relationship exists, and one variable increases as the other decreases. If the correlation is zero, no linear relationship exists between the two variables at all. The square of the correlation coefficient, R^2 , can be interpreted as the fraction of the original scatter in one variable that can be explained or predicted in terms of the other.

Multiple correlation coefficient (R)--a measure of the strength of the linear relationship between a dependent variable and two or more other variables. If the dependent variable can be predicted perfectly from the

other variables, then R is one. If the dependent variable has no linear relationship at all with the other variables, then R is zero. The quantity R^2 is the fraction of the scatter in the dependent variable that can be explained or predicted in terms of the other variables.

Linear combination--a variable X_0 is a linear combination of another set of variables $X_1, X_2, \dots, X_n$ if a set of coefficients $A_0, A_1, A_2, \dots, A_n$ exist such that $X_0 = A_0 + \sum_{i=1}^n A_i X_i$.

Multicollinearity--a certain condition which affects the accuracy of the results of a regression analysis. In the simplest case, multicollinearity exists if two predictor variables are highly correlated. In source receptor modeling, this occurs if two sources have very similar signatures. In a more general sense, multicollinearity exists if any predictor is nearly a linear combination of any subset of the other predictors. When strong multicollinearities are present, conventional regression techniques typically produce results with large uncertainties.

Variance inflation factor--a measure of the effect of multicollinearity on a regression coefficient. A variance inflation factor is the increase in the error variance of a specific regression coefficient due to the effect of multicollinearity alone. If the variance inflation factor for a particular coefficient was one, this would indicate that that coefficient was not affected by multicollinearity at all.

Ridge regression--a type of regression analysis which is specifically designed to handle cases affected by multicollinearity. In CMB analyses, ridge regression has enhanced ability to perform apportionments among sources whose aerosols are chemically similar. However, apportionment among sources whose aerosols are chemically indistinguishable is not feasible even with ridge regression. See the discussion in Section 2.2.

Bias--a systematic as opposed to a random error.

1.3 Overview of Use of Interactive Source Apportionment Software

This report documents an interactive computer program which can be used to perform source apportionment analyses. In each interactive session, one or more separate source apportionments can be performed at the option of the user. A brief overview of the procedures for using the program is presented here. The overview is summarized in Figure 1-2. The procedures are discussed in detail in Section 3.

Before an interactive session, the required input data must be prepared. The following five data files are required:

- List of Source Codes
- List of Species Codes
- Source Signature Matrix (Fine Particulate Fraction)
- Source Signature Matrix (Coarse Particulate Fraction)
- Ambient Particulate Concentration Data

The source code file consists of a numeric code and an alphanumeric code for each source. The species code file requires similar information for each chemical species included in the analysis. These files are used only for labeling and indexing purposes. The source signature and ambient concentration data are used directly in the calculations.

An interactive session has two phases. The first is the initialization phase, which consists of a series of queries and prompts from the program that require responses from the user. In this phase, the user selects the initial set of sources and chemical species to be considered.

In the second phase, the program prompts the user to enter commands. In response to some commands, the program queries the user for additional

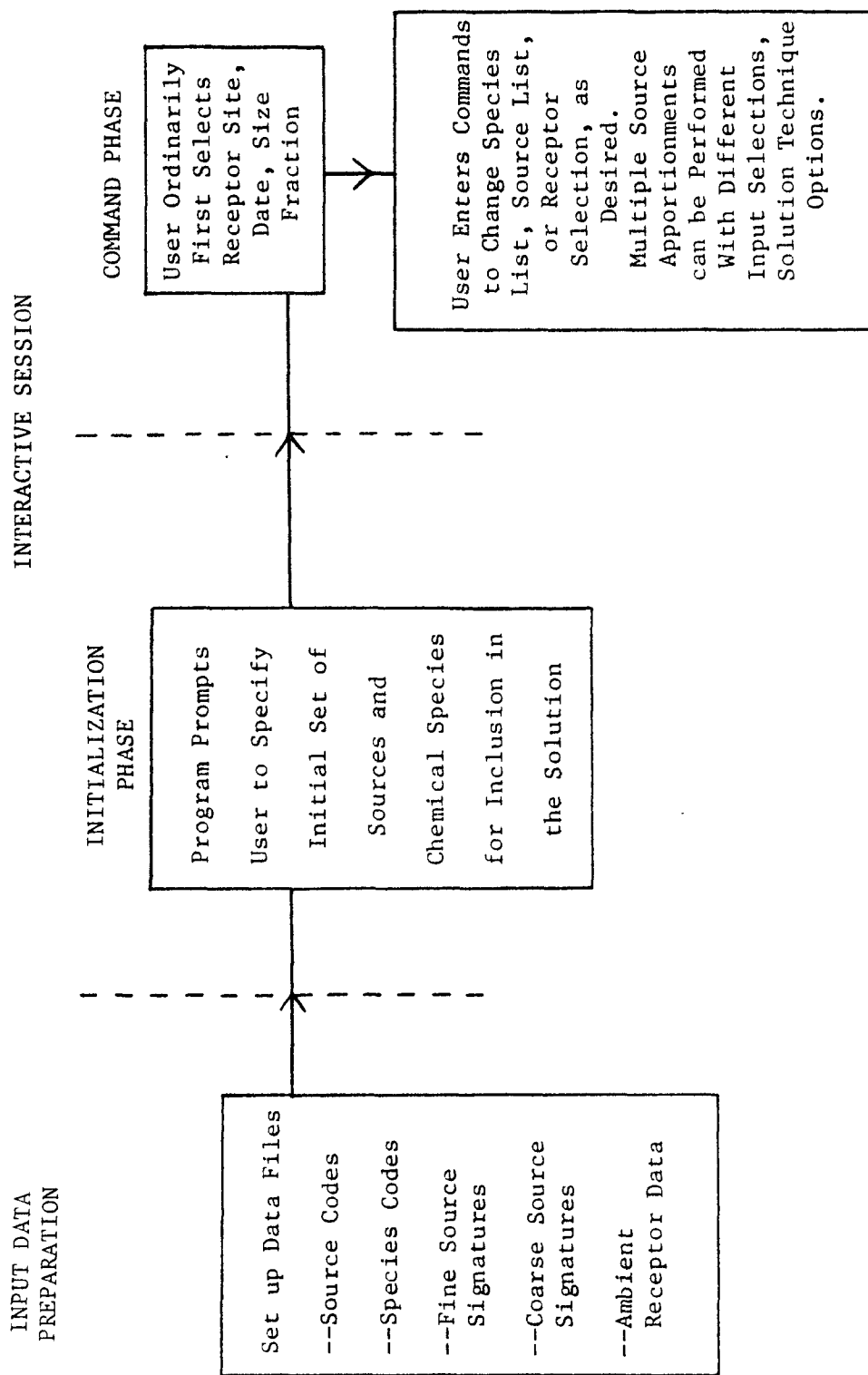


Figure 1-2. Conceptual Flowchart of Activities Involved in Performing Source Apportionments

information. Every command and the associated subsequent queries are discussed in Section 3. Additionally, the HELP command causes the program to list all the commands and give a brief statement of the purpose of each one.

In the command phase, the user ordinarily first selects the site, date, and size fraction (fine or coarse) of the ambient particulate concentrations to be used. It is possible later to alter the initial source or chemical species list. The CMB command causes the computer program to perform a source apportionment analysis using the current ambient receptor site, date, and size fraction and the current lists of chemical species and sources. Various options are available regarding the solution technique.

After a source apportionment is completed, additional problems can be set up by changing the site, date, size fraction, list of sources, list of chemical species, or solution technique. It is possible to perform one or a long series of source apportionment analyses in a single interactive session.

The principal output from a source apportionment consists of:

- (1) an estimate of the contribution of each source to the ambient aerosol concentration, and
- (2) the standard errors, i.e., the uncertainties of those estimates.

Additional statistics are also presented to aid the user in interpreting the results. Outputs from sample problems are presented in Section 4.

In some instances, source apportionment analyses are performed for the fine and coarse fractions for the same date and site and the same lists of species and sources. In these cases, it is possible to command the program to combine the fine and coarse results to produce a source apportionment of the total particulate concentration.

A post-processor program is also available. The post-processor is used to compute mean values and other summary statistics for a series of source apportionments. This feature could be used, for example, if source apportionments had been performed for a set of dates for the same site.

SECTION 2

CONCEPTUAL DISCUSSION OF SOURCE APPORTIONMENT

This section presents a conceptual discussion of source apportionment. The objective here is to provide the user with the technical background needed to use the source apportionment software. Equations are presented only to the extent that they are necessary to explain the basic concepts. The source apportionment problem is discussed in Section 2.1. The solution techniques are discussed in Section 2.2. The mathematical details are presented in Appendix D. The inputs to the computer program and the various options are presented more formally in Section 3.

2.1 Conceptual Discussion of the Source Apportionment Problem

This subsection presents a conceptual discussion of the source apportionment problem. The first step is to define the basic mass balance equation used. This equation establishes the relationship between the required inputs and the outputs and serves as a basis for further discussion.

The standard equation used in CMB analysis is as follows:

$$C_i = \sum_{j=1}^m F_{ij} S_j \quad (1)$$

where

C_i is the ambient particulate concentration of chemical species i ,

F_{ij} is the fraction of the particulate matter emitted from source type j comprised of species i ,

S_j is the ambient particulate concentration resulting from source j , and

m is the number of sources.

The set of values F_{ij} , $i=1, 2, \dots$, is the source signature for source j . This vector of values quantifies the chemical composition of the aerosol from that source. Suppose, for example, that the species Al, Si, K, Ca, Ti, and Ni were being used in the analysis. A small set of elements has been selected for illustrative purposes.

Also, suppose that the soil in the area being analyzed consisted of 5.6% Al, 20% Si, 1.9% K, 2.6% Ca, 0.32% Ti, and 0% Ni. Then the following would be the source signature for soil (assume that soil is source number j_o):

$$\begin{aligned} F_{1j_o} &= 0.056 \\ F_{2j_o} &= 0.20 \\ F_{3j_o} &= 0.019 \\ F_{4j_o} &= 0.026 \\ F_{5j_o} &= 0.0032 \\ F_{6j_o} &= 0 \end{aligned} \tag{2}$$

Notice that the percents have been converted to decimal fractions. The chemical species can be ordered in any way desired, as long as the ordering is the same for all signatures and for the C_i values.

The equation given above is a mass balance equation, as can be explained as follows. The right side of the equation is the sum of a set of terms of the following form: $F_{ij}S_j$. But $F_{ij}S_j$ is the ambient concentration of species i attributable to source j . This fact is illustrated through the following numerical example.

Suppose that soil accounted for $40 \mu\text{g}/\text{m}^3$ of ambient particulate matter, i.e., $S_{j_o} = 40$. From the source signature, we know that windblown dust is 20% silicon. Thus, the ambient concentration of silicon due to windblown dust is

$$(F_{2j_o})(S_{j_o}) = (0.20)(40 \mu\text{g}/\text{m}^3) = 8 \mu\text{g}/\text{m}^3 \tag{3}$$

Thus, the equation

$$C_i = \sum_{j=1}^m F_{ij} S_j \quad (4)$$

simply states that the ambient concentration of chemical species i equals the concentration due to source one plus the concentration due to source two, etc. In other words, the basic equation used is a mass balance equation.

It is possible to add an intercept term S_o to the standard equation:

$$C_i = S_o + \sum_{j=1}^m F_{ij} S_j \quad (5)$$

The term S_o is not indexed since it has the same value in each mass balance equation. The term S_o represents a discrepancy between the measured concentration C_i and the sum of its parts. If all important sources are included and there are no severe data errors, the value of S_o should be small, less than $0.05 \mu\text{g}/\text{m}^3$ in most applications. Thus, including the term S_o simply provides a check. However, it is not required that it be included.

It is also possible to include a mass balance equation corresponding to the total aerosol concentration C_T for the size fraction being analyzed. This equation has the form

$$C_T = S_o + \sum_{j=1}^m S_j \quad (6)$$

This equation states that the aerosol concentration is the sum of the intercept and the contributions of the m sources. The intercept S_o , discussed above, is uniformly included in or excluded from all mass balance equations, including this one.

Note that the mass balance equation involving C_T has exactly the same form as the others. It can be written

$$C_T = S_o + \sum_{j=1}^m F_{i_T j} S_j \quad (7)$$

where

$$F_{i_T j} = 1 \text{ for all values of } j.$$

The quantity i_T is the value of the i index for the equation for the aerosol concentration.

The basic chemical inputs required in CMB analysis include:

- (1) the vector of concentrations, C_i , $i=1$ to n , and C_T ,
- (2) the source signature matrix, F_{ij} , $i=1$ to n , $j=1$ to m , and
- (3) depending on the type of statistical analysis to be performed, the standard errors of the C_i and F_{ij} values.

The unknown quantities in the CMB problem are the S_j values, $j=1$ to m , and the intercept S_0 , if it is included.

The sample size is $n+1$, since there is one observation for each chemical species and one observation corresponding to C_T . Generally speaking, increasing the sample size improves the accuracy in the final results of any statistical analysis, since there is a greater opportunity for errors to balance or average out. While chemical species which serve as tracers for specific sources are generally the most helpful, species which appear in the aerosols from several sources should not be excluded. In any case, the sample size must exceed the number of quantities to be estimated, $m+1$ if the intercept is included and m if not. Having a larger sample size also allows more accurate estimates of the standard errors of the source contributions. As in any regression analysis, if the number of regression coefficients estimated was almost as large as the sample size, the standard errors could be artificially low and the R^2 value could be artificially high. Further discussion of the standard errors is presented below and in Appendix D.

There is no reason why all chemical species present in the ambient aerosols have to be included in the analysis. However, it is important to include all important source types. If a major source was inadvertently left out, its aerosol contribution would probably be apportioned among the

sources that were included. The sources whose signatures were most similar to that of the omitted source would be increased by the greatest amount.

Within a given CMB analysis, two sources can be distinguished only if they have different source signatures. Thus, each of the m "sources" included is actually a category of sources which have the same or very similar source signatures. The categories can include natural sources, such as soil and, if appropriate, sea salt, and anthropogenic categories, such as automobiles, petrochemical plants, coal-fired power plants, cement production, etc.

A single CMB analysis alone can not differentiate among the sources within a category. For example, the aerosol contribution of cement production could be estimated, but the separate contributions of each cement facility would not be quantified. However, inferences about the effects of individual sources can be drawn in some instances from wind information. It is sometimes helpful to perform several separate analyses of cases with different wind directions.

Whenever possible, it is beneficial to subdivide source categories to produce more resolution in the final source apportionment. For example, automobiles with and without catalytic converters can be treated as two separate sources, since their aerosols are chemically different. Determining the appropriate set of source categories in a given situation can be a subtle problem. It is discussed further in the following subsection.

Another issue involves the handling of secondary aerosols. One approach is to treat secondary aerosols, especially sulfates and nitrates, as separate "sources." In the source signature for sulfate, for example, all entries would be zero except the one corresponding to SO_4 , and this entry would be one; i.e.:

$$\begin{aligned} F_{ij_0} &= 0, \quad i \neq i_0, \quad \text{and} \\ F_{i_0j_0} &= 1 \end{aligned} \tag{8}$$

where

j_o is the source index corresponding to secondary sulfate, and
 i_o is the chemical species index corresponding to SO_4 .

If the elemental S concentration were used rather than SO_4 , then the scheme above would be employed, except i_o would be the chemical species index corresponding to S. In the above, it is assumed that not both S and SO_4 are included in the same analysis.

In most applications, ambient concentrations are available for a series of sampling periods. There are several ways in which these data can be employed. First, a separate CMB analysis could be performed for each sampling period. This approach is beneficial if a separate source apportionment for each period is needed. Subsequently, averaging of the CMB results can be performed. In most such applications, the same source signature matrix would be used for all periods. Thus, whatever errors are present in the source signatures are common to all periods. Therefore, the separate solutions have correlated errors.

The upshot of this is as follows. Suppose a set of values $S_j^1, S_j^2, \dots, S_j^H$ are obtained for S_j for H sampling periods. The value S_j^h is the aerosol contribution of source j in the h^{th} sampling period, $1 \leq h \leq H$. The conventional mean value $\bar{S}_j$

$$\bar{S}_j = \frac{1}{H} \sum_{h=1}^H S_j^h \quad (9)$$

is an unbiased estimate of the average aerosol contribution of source j during the study period. However, the conventional standard error of the mean

$$s_m = \left[\frac{1}{H(H-1)} \sum_{h=1}^H (S_j^h - \bar{S}_j)^2 \right]^{\frac{1}{2}} \quad (10)$$

is low-biased due to the correlated errors in the individual S_j^h values.

The regression analysis for period h produces the estimate S_j^h and the corresponding standard error s_{jh} . Another approach is to use error propagation techniques to compute the standard error of $\bar{S}_j$ in terms of the s_{jh} values, $1 \leq h \leq H$:

$$s'_m = \frac{1}{H} \left[\sum_{h=1}^H s_{jh}^2 \right]^{\frac{1}{2}} \quad (11)$$

However, this approach fails for the reason discussed above. The quantity s'_m would be an unbiased estimate of the standard error of $\bar{S}_j$ if the errors in the individual S_j^h values were independent. Due to the positively correlated errors, however, s'_m has a low bias.

There is an alternative method for obtaining the average contributions of the different sources and the corresponding standard errors. The approach involves averaging the concentrations of each C_i and C_T separately, just as the S_j^h values are averaged above. Then a single CMB analysis can be performed for the entire study period using the averaged concentrations. The standard errors of the results will be produced by conventional regression analysis procedures. These standard errors will not be affected by the correlated error problem discussed above.

It is also possible to average data in groups and perform a separate CMB analysis for each group. For example, in a given application, one might average all data taken at sites downwind of a given city when the wind was persistently from the north. The groups are usually selected on the basis of meteorological conditions and spatial relationships.

2.2 Conceptual Discussion of Statistical Solution Techniques in CMB Analysis

This subsection presents a conceptual discussion of the solution techniques available for CMB analysis. The basic approach employed in the computer program documented herein is regression analysis. However, several

additional features are also provided to handle specific aspects of the problem. These features include the following:

- (1) Weighted least squares--a modification of conventional regression in which the more accurate concentration data are weighted more heavily to produce a better solution. Weighted least squares is a standard feature of the program, not an option.

The following two features are options:

- (2) Effective variance calculations--a modification of weighted least squares in which the uncertainties in the source signatures as well as the uncertainties in the concentration data are taken into account.
- (3) Ridge regression--a technique designed to handle cases with similar source signatures.

It is possible to select either option (2) or (3), both of them, or neither.

The discussion of the statistical methods presented here is designed to help the user select the appropriate method for his problem. The mathematical details are given in Appendix D.

The basic CMB equations

$$C_i = S_o + \sum_{j=1}^m F_{ij} S_j \quad (12)$$

are linear in the S_j values. Thus, a solution could be obtained through linear regression analysis. In the terms of regression analysis, the C_i 's are the values of the dependent variable, F_{ij} is the i^{th} value of the j^{th} predictor variable, S_o is the intercept, and S_j is the j^{th} regression coefficient.

The solution by conventional least squares is accomplished by choosing S_o and the S_j values to minimize the sum of squares of the differences between the left and right sides of the mass balance equation above:

$$\sum_i (\hat{C}_i - C_i)^2 + (\hat{C}_T - C_T)^2 \quad (13)$$

where

$$\hat{C}_i = S_o + \sum_{j=1}^m F_{ij} S_j \quad (14)$$

and

$$\hat{C}_T = S_o + \sum_{j=1}^m S_j \quad (15)$$

i.e., $\hat{C}_i$ and $\hat{C}_T$ are the estimated or calculated concentrations, and C_i and C_T are measured concentrations.

In conventional least squares, all data are weighted equally in the calculations. This is acceptable if the uncertainties of all the data are about the same. In weighted least squares, the more accurate data are weighted more heavily to produce a more accurate solution. In weighted least squares, S_o and S_j values are selected to minimize the following:

$$\sum_i \frac{(\hat{C}_i - C_i)^2}{s_{C_i}^2} + \frac{(\hat{C}_T - C_T)^2}{s_{C_T}^2} \quad (16)$$

where

s_{C_i} is the standard error of C_i , and

s_{C_T} is the standard error of C_T .

Weighted least squares employs the uncertainties of the concentration data only. However, the source signature data also have uncertainties. It is possible to account for these uncertainties also by using effective variances (Watson, 1979). The mass balance equation

$$C_i = S_o + \sum_{j=1}^m F_{ij} S_j \quad (17)$$

can be rewritten

$$C_i - S_o - \sum_{j=1}^m F_{ij} S_j = 0 \quad (18)$$

The effective variance $s_{EV_i}^2$ for this equation is the variance of the entire left side of the final equation, including the effects of the errors in C_i and F_{ij} , $j=1$ to m . The exact expression for the effective variance is given in Appendix D. The main point is that the effective variance is an estimate of the total uncertainty in an equation, taking into account the errors in all input data in the equation.

After the effective variances are calculated, S_o and the S_j values are selected to minimize the following:

$$\sum_i \frac{(\hat{C}_i - C_i)^2}{s_{EV_i}^2} + \frac{(\hat{C}_T - C_T)^2}{s_{EV_T}^2} \quad (19)$$

Thus, the effective variance approach involves a weighted least squares analysis but uses refined estimates of the weights.

Appendix D shows that calculation of the effective variances requires estimates of the S_j values, and the S_j values are computed in terms of the effective variances. For this reason, an iterative solution is required if effective variances are used.

Before discussion of the third feature, ridge regression, a few comments will be made about the input standard errors. If blank values were entered for the standard errors of either the ambient concentrations or the source signatures, zeroes would be stored. A weighted regression analysis cannot be performed using species whose concentrations have zero standard errors. If an attempt is made to do such an analysis, the program will print a message and abort that particular source apportionment. Nonzero standard errors are not required, however, for species used only to compare observed

and predicted concentrations but not used in the regression analysis (see Section 3).

The standard errors for the source signatures are used only if the effective variance feature is selected. Zero values for these standard errors would not prevent the analysis from being performed. Moreover, a zero standard error could be correct in some cases. For example, it could be known that a given species was absent from the aerosols from a particular source. Then the signature entry for that source and chemical species would be zero with a standard error of zero.

However, if some zero standard errors were present due to blanks which were entered only because the standard errors were not known, inaccuracies could result. The source signature entries with zero standard errors would be treated as if they were known exactly, while the entries with nonzero standard errors would be treated as having random errors. Thus, the weighting of the data would not be in accordance with the actual uncertainties. As a result, the final results would have larger uncertainties than if the weighting had been performed correctly. The increase in the uncertainties might not be reflected in the calculated standard errors of the final results. If all entries for the source signatures had zero standard error entries, use of the effective variance option would not change the final answers. The only effect of using effective variances in this case would be to increase the computer time somewhat.

The third feature which can be added to the solution technique is called ridge regression analysis. Ridge regression is an advanced statistical technique which is useful when two or more sources have similar signatures. Clearly, if two sources had identical signatures, their contributions to the ambient aerosol could not be separated through CMB analysis. If the signatures were similar but not identical, separation would be possible but difficult to accomplish accurately. The problem is referred to as "multicollinearity." Stated more generally, multicollinearity exists

when any source signature is nearly a linear combination of any subset of the other signatures.

The effect of multicollinearity is to cause large random errors in the estimates of the S_j if conventional techniques are used. If severe multicollinearities are present, it is even possible to obtain negative S_j values with large magnitudes.

The variance inflation factor is a convenient measure of the effects of multicollinearity in a given problem. The variance inflation factor VIF_j is defined as follows:

$$VIF_j = \frac{\text{var}(S_j)}{\text{var}^1(S_j)} \quad (20)$$

where

$\text{var}(S_j)$ is the error variance of S_j if it is calculated through conventional regression techniques, and

$\text{var}^1(S_j)$ is the error variance S_j would have had in the absence of multicollinearity.

Thus, VIF_j is the increase in the uncertainty (error variance) of S_j due to the effect of multicollinearity alone. If S_j was not affected by multicollinearity at all, VIF_j would be one. If VIF_j was near one, say between one and 1.5, one could say that the effect of multicollinearity on S_j was relatively small. Suppose, however, that VIF_j was 100. This would mean that the error variance of S_j was increased by a factor of 100, and the standard error of S_j was increased by a factor of 10, by the effect of multicollinearity alone. It is beneficial to examine the variance inflation factors in each problem to determine whether multicollinearity is a serious factor.

Factor analysis and principal component analysis are additional statistical methods which can be used to analyze the multicollinearities in a given data set. While these methods are outside the scope of this report, they are discussed by Morrison (1967) and other writers on multivariate statistical methods.

If multicollinearities are present, there are basically two approaches. One approach involves first identifying the sources whose signatures are collinear; soil, road dust, and asphalt production ordinarily form such a set. Then one of the sources can be chosen to represent each set. In the example given, this would mean that the combined contribution of soil, road dust, and asphalt production to the ambient aerosol levels would be estimated, but their individual contributions would be unknown. Some combining of sources into categories is usually necessary. However, the greater the number of separate source categories, the greater the resolution is in the source apportionment.

The second approach is to employ ridge regression, a technique which is designed to handle cases affected by multicollinearity. In ridge regression, the goal is to introduce a small bias into the solution in order to achieve a large reduction in the random error, so that the total error (bias plus random error) is reduced.

In ridge regression a parameter k is introduced. The exact mathematical definition of k is given in Appendix D. The important point is that as k increases, the random error decreases and the bias error increases. The objective, then, is to pick a value of k near the optimum, where the total, or bias plus random, errors are minimal. The program computes the solutions for a set of values of k . At the user's option, the program will select a value of k according to criteria given in Appendix D. The user also has the option of displaying the solutions for the complete set of values of k .

The value $k=0$ is included in the set. When $k=0$, the ridge solution is the same as the conventional least squares solution. If this is the best solution according to a specified set of criteria, it can be selected. Thus, using the ridge feature does not prevent the conventional least squares solution from being used, but it allows an additional set of solutions to be considered.

There is presently not an algorithm which guarantees selection of the optimal k value. When multicollinearities are present, the regression coefficients are typically extremely sensitive to k for small values of k . However, as k increases, the coefficients stabilize. Hoerl and Kennard (1970a, b) suggest choosing k from within the stable region, where moderate changes in k do not affect the coefficients significantly. Thus, slight deviation from the optimal k would not cause serious errors.

There is no simple formula which tells the user when sources should be combined into one category and when their separate aerosol contributions should be estimated. However, the variance inflation factor, discussed above, is an objective measure which tells the user which sources are affected by multicollinearity and to what extent.

One rule of thumb which can be used is to determine whether the signatures of two sources differ more than their uncertainties. Theoretically, a significant difference for only one chemical species would be sufficient to allow the user to separate the influences of the two sources. Also, the user should remember that, generally, random errors tend to balance or "average out" in a statistical analysis. Thus, if two source signatures were different by about the uncertainty level for each of several species, it is possible that meaningful separation of the sources could be achieved. The use of as many species as possible in the analysis allows the maximum opportunity for the error averaging effect to occur.

Another approach is to perform different source apportionment analyses with different levels of source resolution and then compare the results. For example, in one analysis, soil and road dust could be combined into a "crustal" source, and in a second analysis they could be treated separately. If the estimates of the separate aerosol contributions for soil and road dust were physically unreasonable or had excessively large standard errors even when the ridge regression was used, this would indicate that the two sources should be combined. However, if the estimates of their separate contributions were physically reasonable and had acceptably small standard errors, then they should probably be treated as two sources. The standard errors of the two separate sources in one analysis should be compared to the standard error for the crustal source in the other.

Regarding the performance of ridge regression, in a survey article on the subject, Vinod (1978) states the following:

Readers of this review are familiar with multicollinearity problems, discussed by Farrar and Glauber (1967), Leamer (1973), and others. Hoerl and Kennard's (1970a, b) ridge regression (RR) offers new hope for avoiding most serious ill-effects of multicollinearity on ordinary least squares (OLS) regression coefficients. These include "wrong signs," drastic changes in regression coefficients after minor data revision or omission of one or two observations, and conflicting conclusions from usual significance tests.

In Monte Carlo experiments the true regression coefficients are specified. The data structure is usually chosen from a real life regression problem. Random numbers are used to create hundreds of "typical" regression problems. The estimated regression coefficients using RR and OLS are compared in terms of mean-squared error (MSE), i.e., the average squared Euclidian distance between the estimate and the parameter. In the following independent studies by investigators from diverse fields, the superiority of RR over OLS [ordinary least squares] is almost always noted; although there is wide disagreement about the "optimum" RR method.

In support of the statements above, Vinod subsequently references sixteen published Monte Carlo studies and refers to "many unpublished dissertations." Selection of the optimum RR method is discussed above.

The quotation above was chosen from the extensive literature on ridge regression because (1) it appears in a survey article and summarizes results from many independent studies and (2) the results to which Vinod refers are objective in nature, being comparisons of true and estimated regression coefficients in Monte Carlo studies. However, no single quotation could represent all opinions expressed in the literature. In the following quotation, Draper and Smith (1981) present another view regarding the simulation results. They use the letter " θ " to denote the ridge parameter, referred to as "k" here.

Ridge Regression Simulations--A Caution

A number of papers containing simulations of regression situations claim to show that ridge regression estimates are better than least squares estimates when judged via mean square error. Such claims must be viewed with caution. Careful study typically reveals that the simulation has been done with effective restrictions on the true parameter values--precisely the situations where ridge regression is the appropriate technique theoretically. The extended inference that ridge regression is "always" better than least squares is, typically, completely unjustified.

Summary

From this discussion, we can see that use of ridge regression is perfectly sensible in circumstances in which it is believed that large β -values are unrealistic from a practical point of view. However, it must be realized that choice of θ is essentially equivalent to an expression of how big one believes those β 's to be. In circumstances where one cannot accept the idea of restrictions on the β 's, ridge regression would be completely inappropriate.

Note that, in many sets of data, where the sizes of the least squares estimates are acceptable as they are, the ridge trace procedure would result in a choice of $\theta = 0$. A value of $\theta \neq 0$ would be used only when the least squares results were not regarded as satisfactory.

There is a large and growing literature on the many aspects and generalizations of ridge regression; some selected references are given at the end of the book.

OPINION. Ridge regression is useful and completely appropriate in circumstances where it is believed that the values of the regression parameters are unlikely to be "large" (as interpreted through σ_{β}^2 or c^2 above). In viewing the ridge traces, a subjective judgment is needed which either (1) effectively specifies one's Bayesian prior beliefs as to the likely sizes of the parameters, or (2) effectively places a spherical restriction on the parameter space. The procedure is very easy to apply and a standard least squares regression program could easily be adapted by a skilled programmer. Overall, however, we would advise against the indiscriminate use of ridge regression unless its limitations are fully appreciated. (The reader should be aware that many writers disagree with our somewhat pessimistic assessment of ridge regression.)

Draper and Smith have indicated that ridge regression is "perfectly sensible in circumstances in which it is believed that large β -values [regression coefficients] are unrealistic from a practical point of view." They also say that "In circumstances where one cannot accept the idea of restrictions on the β 's, ridge regression would be completely inappropriate." Recall from the discussion above that the regression coefficients are the estimates of the source contributions.

The question, then, is whether a priori knowledge exists in source apportionment applications which would allow coefficients with unreasonably large magnitudes, if present, to be identified. The answer to this question is yes. Consider the case in which the signatures of two or more sources are collinear. Typically, if conventional weighted least squares is used, one of the collinear sources will have a large positive error, and another source will have a counterbalancing negative error with large magnitude. The large errors cause the regression coefficients with large magnitudes referred to by Draper and Smith. The following are two useful criteria for identifying this situation in source apportionment applications:

- (1) In extreme cases, one of the estimated source contributions may exceed the aerosol concentration for the size fraction being analyzed. The existence of an upper bound for contributions from individual sources provides one criterion for identifying

excessively large coefficients. To be conservative one could use the aerosol concentration plus three times its standard error as the upper bound.

- (2) If multicollinearities are present, the counterbalancing negative errors mentioned above can cause negative estimates of some source contributions. If negative estimates with large magnitudes were present, the solution would clearly be physically unreasonable.

Thus, both an upper bound (the aerosol concentration for the size fraction being analyzed) and a lower bound (zero) exist for the regression coefficients. If either of these bounds was significantly exceeded, the solution should be considered unreasonable. Source apportionment, then, is a context in which criteria exist for recognizing unreasonably large regression coefficients. Thus, according to Draper and Smith's discussion, ridge regression should be considered a useful tool in source apportionment applications. The authors of this report feel that the use of ridge regression in a given problem can also be justified on other grounds, such as the presence of large variance inflation factors and sensitivity of both the regression coefficients and their standard errors to k , especially for small values of k .

However, Draper and Smith are right that ridge regression should not be used indiscriminately, as if its application would automatically eliminate all problems caused by multicollinearity. As is indicated by both articles, it cannot be guaranteed that ridge regression will produce a better solution in every application than does conventional least squares. It should also be remembered, however, that use of the ridge option does not prevent selection of the solution for $k=0$ if this solution is the best. The solution for $k=0$ is equivalent to the weighted least squares solution.

SECTION 3

GUIDE TO USE OF INTERACTIVE SOURCE APPORTIONMENT SOFTWARE

This section discusses the procedures required to use the interactive source apportionment software. One or more source apportionment analyses can be performed in a single interactive session.

There are three types of inputs to the CMB program:

- Data Files

- Commands

- Responses to Queries

The data files, which contain the source signatures, ambient concentration data, and other information, must be set up before an interactive session is begun. Commands and responses are entered interactively. The user may enter any of the allowed commands following the prompt "ENTER COMMAND." Responses to queries are the user replies to specific questions or data requests from the CMB program.

There are five input data files that are required by the program:

- List of Source Codes

- List of Species Codes

- Source Signature Matrix (Fine Particulate Fraction)

- Source Signature Matrix (Coarse Particulate Fraction)

- Receptor Concentration Data

A certain degree of incompleteness is possible. For example, if only fine fraction data are available for source signatures, an empty data file is acceptable for the coarse fraction.

An interactive session with the CMB program consists of two phases: an initialization phase and a command phase. The program controls the

initialization phase by prompting the user for the initial sources and species. The user may add or delete sources and species for either size fraction in the working phase. The user controls the command phase by issuing commands. The command may be performed immediately or the CMB program may prompt the user for additional information before proceeding. The user must spell out the command in full. However, responses to prompts from the computer may be abbreviated by the first letter of the response unless a numerical value or alphanumeric code (site code) is requested. For example, a "Y" has the same effect as "YES." In fact, the program reads only the first letter of nonnumeric, non-code responses. Thus, "SOURCE SIGNATURE" can be abbreviated "SOURCE" or "S."

In the following subsections, discussions are presented on the following:

- (1) required data files,
- (2) initialization phase of the interactive session,
- (3) command phase of the interactive session,
- (4) formats of required data sets,
- (5) command reference summary, and
- (6) computer system considerations .

3.1. Description of Data Files

The CMB program requires 11 files for input or output. These include data input files, hardcopy printout files, interactive communications, and temporary data storage files. These files are accessed by the CMB program according to the following FORTRAN Input/Output unit numbers:

<u>Unit #</u>	<u>Purpose</u>	<u>I/O</u>
2	Source Names/Codes	Input
3	Species Names/Codes	Input
5	Interactive Read	Input
6	Interactive Write	Output
7	Fine Fraction Signature	Input
8	Coarse Fraction Signature	Input
9	Hardcopy Print (Summary)	Output
10	Temporary Storage	Input/Output
11	Hardcopy Print (General)	Output
12	User-Followup Data	Output
13	Receptor Concentrations	Input

The user's terminal serves as the interactive read and write units. The user's commands and replies are read and the program's queries and output are written. The program output includes the fitted CMB coefficients and predicted concentrations. Sections 3.2 and 3.3 describe the commands, queries and replies. Section 4 presents an annotated interactive session.

3.1.1 Input Data Files

There are five input data files that must be available to the program before an interactive session can begin. The purpose and content of each data file are described below. The detailed record formats are given in Section 3.4, and examples are given in Appendix C.

The source and species names are for the convenience of the user. The source and species codes must be consistent across all data sets. These codes are used for labeling the data sets only. During the interactive session the program will assign source and species numbers that may not agree with the source and species codes. The source and species numbers, not the codes, must be used in the interactive session. The source and species numbers can be listed at the beginning of the interactive session. The source and species codes and numbers, the source signature matrix, and the current receptor concentrations can be listed with the PMATRIX command during an interactive session.

The following are descriptions of the required input files:

Source and Source Code List--Eight-character source names and two-digit source codes are required. The source signature matrix must be coded consistently with this list. The two-digit codes may range from "01" to "99" in any order. Gaps are allowed in the code range. Sources not used in the current source signature matrix can be present. The maximum number of sources which can be included in the input data files is 35.

The maximum number of sources which can be included in a given CMB analysis, however, is 16.

Species and Species Code List--Eight-character species names and two-digit species codes are required. The source signature matrix and the receptor concentrations must be coded consistently with this list. The same comments made for source codes apply here. The maximum number of species which can be included in the input data files is 35. The maximum number of species which can be used in a given CMB analysis is 21.

Fine Fraction Source Signature Matrix--The fraction of the aerosols from each source accounted for by each species is required. If the effective variance method is to be used, the standard error of each item is also required. Each item and its standard error are entered on a separate line (record or card) along with the identifying source and species codes.

Coarse Fraction Source Signature Matrix--The same comments as for the fine fraction apply here.

If coarse fraction data are not available, a dummy data set may be substituted.

Receptor Concentration Data--The receptor concentration and its standard error are required for each species for both fine and coarse fractions. Alternatively, the fine fraction and total aerosol may be substituted and the program will calculate the coarse fraction data. Each species is coded on a separate line (card or record).

If only fine fraction data are available the coarse fraction may be coded as zero.

3.1.2 Output Data Files

The CMB program writes to three permanent files: the general hardcopy, the summary hardcopy, and the user followup data file. The two hardcopy files are for printed results (132-character line). The postprocessor data file makes certain input and output data available for further processing. Examples are given in Appendix C.

General Hardcopy--The general hardcopy printout includes hardcopy versions of results displayed in the interactive sessions. Some additional calculated values are presented that are not included in the terminal displays. The primary output to the general hardcopy is the display of CMB coefficients with measured and calculated concentrations. Appropriate standard errors, percentages, and ratios are included. This output results from a WRITE command.

Certain other commands can direct results to the general hardcopy. The PMATRIX command prints input matrices. The PSOLN command prints ridge regression solutions. The PCOMP command prints averages of source contributions.

Summary Hardcopy--The summary hardcopy printout tabulates the CMB coefficients for fine, coarse and total fractions. Standard errors and percent composition are included. This report is printed by the WRITE command only when both fine and coarse fractions are analyzed for the same site and date.

User Followup Data File--The user followup data may be used for further analysis with user-written software. The calculated concentration of each species contributed by each source is written to this file. The program writes these values to the file by the WRITE command only when both fine and coarse fractions are analyzed for the same site and date (as with

the summary hardcopy). The measured concentrations are also placed on the file. The detailed format of the data file is given in Section 3.4.

3.2 Initialization Phase of an Interactive Session

The initialization phase consists of a series of queries and prompts from the program that require responses from the user. Most of the required responses are to identify the sources and species. Each query is given below followed by a discussion of the appropriate user response.

WOULD YOU LIKE TO LOOK AT THE SOURCE AND SPECIES LISTS?

Unless the user is familiar with the program and data, he should reply "YES." If the user responds "YES" the program lists the sources and species by number and name at the terminal. In other parts of the session the user will be asked what sources or species he wants to add, delete, or display. The user must respond with the source or species number according to these lists. Generally, the program will display the source or species number along with the name whenever it appears.

PLEASE INPUT INITIAL FITTING INFORMATION

INITIAL SOURCE 1: XX

At this point the user tells the program which sources to include in the initial problem set. The user should key in the desired source numbers, one line at a time in response to the program prompts, "INITIAL SOURCE 1: XX," "INITIAL SOURCE 2:XX," and so forth. When all of the desired sources have been entered, the user should reply with a blank or null line (carriage return with no data).

If the user wants all the available sources in the initial problem set, he should enter "-1" and the program will automatically include them up to its limit, which is 16. The user can also use this feature to save time

when almost all sources are wanted. The DS (Delete Source) command can be used later to remove unwanted sources.

PLEASE INPUT SPECIES

INITIAL SPECIES 1:XX

At this point the user tells the program which sources to include in the initial problem set. The above discussion for entering initial sources applies also to species. The DE (Delete Species) command can be used later to remove unwanted species.

ARE INITIAL SOURCES AND SPECIES CORRECT?

If the user responds "YES," then the session enters the command phase. The program responds with "ENTER COMMAND" (see below). If the user responds "NO," then he is prompted with the following query:

USE COMMANDS AE, DE, AS, DS FOR CHANGES.
OR, DO YOU WANT A FRESH START?

Both fine and coarse size fractions will start with the initially chosen sources and species. The user can use the add and delete commands to change the list of sources and species for either size fraction. Later the user can restore either size fraction to the initially chosen sources and species. A "YES" response to this query returns the session to "PLEASE INPUT INITIAL FITTING INFORMATION" to re-enter the initial choice of sources and species. A reply of "NO" gets the following prompt:

THE HELP COMMAND LISTS COMMANDS
SIZE IS FINE
ENTER COMMAND

The session has entered the command phase. This phase is discussed in the next section. The size fraction is currently set to "fine."

3.3 Command Phase of an Interactive Session

The command phase of the CMB program is indicated by the prompt "ENTER COMMAND." Each command is invoked by entering its name in the keyboard. For some commands this is all that is necessary. Other commands will prompt the user for additional information.

During the command phase many parameters remain set at previous values until changed by the user. This feature relieves the user from the repetitive entries that would otherwise be necessary. The parameters that hold their values and the commands that change them are the following:

<u>Parameters</u>	<u>Commands to Change</u>
List of Sources	AS, DS, INITIAL
List of Species	AE, DE, INITIAL
Receptor Concentrations	SELECT, AUTOFIT
Size Fraction	SIZE, SELECT, AUTOFIT
Background	BACKOUT, BACKIN

The command "PINFO" will display the current status of these parameters.

3.3.1 HELP

The HELP command lists all the commands with a brief statement of the purpose of each one.

3.3.2 SELECT

The SELECT command is used to select the receptor data for the current problem. SELECT also automatically invokes commands CMB and PDATA. Under normal use, SELECT will be the first command of the interactive session.

SELECT will prompt the user to identify the receptor data as follows:

ENTER DESIRED CMB SITE CODE: XXXXXXXXXXXX

The user should respond with the site code or name. If the sites available are not known, enter a "?" or "Q" and then give blank responses to the next three queries. The program will list the available receptors and dates for which data are available. Subsequently, the user can use the SELECT command again and choose a site and date from those listed.

ENTER YEAR: YY

Key in the last two digits of the desired year.

ENTER DATE: MMDD

Key in the month and day numbers of the desired sampling date. For example, June 26 is 0626.

INPUT DESIRED SIZE FRACTION: (FINE OR COARSE)

Key in FINE for the fine fraction or COARSE for the coarse fraction.

The CMB program will now search the receptor concentration data set for the desired data. As it does so it will display the cases it encounters

in the search. At the far right will be the letters FC for Fine/Coarse data type or FT for Fine/Total data type. The portion not present will be calculated.

The program then begins the CMB command followed by PDATA.

3.3.3 CMB

The CMB command performs the analysis. It also prompts the user for the various method options. The method options are:

Weighted Ridge Regression/Weighted Least Squares

Effective Variance Method/No Effective Variances

Fitted Model Intercept/Zero Intercept

These options may be exercised in any combination.

DO YOU WANT RIDGE SOLUTIONS?

Reply "YES" for weighted ridge regression or "NO" for weighted least squares. (Reply "SAME" for the same method options chosen in the previous use of the CMB command. The program will then proceed directly to the analysis without further queries.) If the reply is "YES" then the following two queries will be presented:

CMB WILL SELECT THE BEST RIDGE SOLUTION

DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?

A "YES" response will cause the program to display the following items for each ridge k-value: R^2 , calculated total aerosol (sum of coefficients), negative coefficient of greatest magnitude, the number of negative coefficients, and the number of iterations. If the effective variance option is not used, the number of iterations is always one.

IN THE SELECTION OF THE BEST RIDGE SOLUTION, WHAT WEIGHT DO YOU WANT?
(DEFAULT = 1.0)

In the selection of the best ridge solution two criteria are considered: closeness of the calculated aerosol total to the measured aerosol total and the smallness in magnitude of any negative coefficients. These two criteria are weighted in choosing the best solution. A weight of 1.0 gives an "even" weight to the two criteria. A weight less than 1.0 gives more weight to the closeness of the total aerosol calculated and measured values. A weight greater than 1.0 gives more weight to the smallness in magnitude of any negative coefficients. The mathematical details for the selection of the ridge solution are discussed in Appendix D.

Key a null line (press return) for the default weight 1.0. Otherwise, enter a number above zero but less than ten million. The decimal point must be keyed.

DO YOU WANT TO USE EFFECTIVE VARIANCES?

A "YES" reply will invoke the effective variance method. Standard errors must be present on the source signature matrix. Reply "NO" if the effective variance method is not desired.

DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?

A "NO" reply sets the intercept to zero. A "YES" reply allows the program to fit the intercept to the data. A fitted intercept value greatly different from zero is an indicator of difficulties. This may result from an important source being omitted or data errors.

The CMB program now performs the analysis. If the effective variance and ridge options are in effect, the following prompt may occur, particularly for the first ridge k-value (zero or least squares):

XXX ITERATIONS SO FAR FOR RIDGE K = X.XXX WITHOUT CONVERGENCE. HOW MANY MORE DO YOU WANT TO TRY?

If the effective variance option is in effect but the ridge option is not, the following prompt may occur:

XXX ITERATIONS SO FAR WITHOUT CONVERGENCE. HOW MANY MORE DO YOU WANT TO TRY?

Reply with the number of extra iterations. Generally, just a few more are required (less than 10). If no more iterations are wanted key a zero, and the solution will be the current estimate.

The program now enters the PDATA command automatically.

3.3.4 PDATA

The PDATA command displays the problem solution at the user's terminal. The output consists of the solution coefficients and standard errors. The least squares solution is automatically printed along with variance inflation factors. This means that the same solution will be given twice if the ridge regression option is not used.

Optionally, the actual and calculated receptor concentrations will be displayed:

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND

A null line (press the transmit or enter key) will result in the optional receptor concentration display. Key in a C if this information is to be suppressed.

The output from PDATA can be sent to hardcopy with the WRITE command.

3.3.5 WRITE

The write command writes the solution and other information to storage files for later use or display. The files to which data are written are:

General Hardcopy

Summary Hardcopy

User Followup Data, and

Temporary Storage for use by the PCOMP command.

The hardcopy files may be printed at the user's terminal or on the system printer after the end of the CMB interactive session. Section 3.6 discusses access to these files.

The report written to the general hardcopy is an expanded version of the terminal display given by the PDATA command. The report written to the summary hardcopy is a summary of these reports for fine, coarse and total sizes. The items written to the user followup data file are contributions from each source to the calculated concentration of each species.

The WRITE command writes the current CMB analyses results to the general hardcopy file. This is confirmed at the user's terminal by the message "WRITTEN." The WRITE command writes to the summary hardcopy, the user followup data, and the temporary storage only under the following conditions: both fine and coarse CMB analyses are performed in succession and each is followed by a WRITE command. The same site and date must be used for both size fractions. This occurrence is confirmed at the user's terminal by two successive "WRITTEN" messages. A CMB analysis display for the total of the fine and coarse fractions is also written to the general hardcopy at this time.

Section 3.1.2 discusses the contents of the three output files. Section 3.4 gives the format of the user followup data file. Appendix C gives examples of the output to these files. A flow diagram illustrating the WRITE command is given in Appendix B.

3.3.6 SIZE

The SIZE command changes the size fraction from the current setting to the other. (The two alternatives are fine and coarse.) The command then displays the new current size fraction.

3.3.7 AE

The AE command is used to add species to the current working list. The program prompts the user for species to add. The user responses are checked for validity. After the AE command is made, the user is prompted with the following:

```
SIZE IS XXXXXX  
INPUT CODE OF ADDED SPECIES
```

The user should reply with the species number. The program will then issue the prompt again and another species may be added. When all species desired are added, give a blank or null line (press transmit or enter).

If the entry is invalid or unintelligible the program will print a message and issue a new prompt.

If the current size fraction displayed is not the desired one, then the user should terminate the command (enter a blank line), give the SIZE command, and re-enter the AE command.

3.3.8 DE

The DE command is used to delete species from the current working list. The program prompts the user for species to delete. The user responses are checked for validity. After the DE command, the user is prompted with the following:

SIZE IS XXXXXX

INPUT CODE OF DELETED SPECIES

The user should reply with the species number. The program will then issue the prompt again and another species may be deleted. When all species desired are deleted, give a blank or null line.

If the entry is invalid or unintelligible the program will print a message and issue a new prompt.

If the current size fraction displayed is not the desired one, then the user should terminate the command (enter a blank line), give the SIZE command, and re-enter the DE command.

3.3.9 AS

The AS command is used to add sources to the current working list. This command functions similarly to AE.

3.3.10 DS

The DS command is used to delete sources from the current working list. This command functions similarly to DE.

3.3.11 INITIAL

The INITIAL command restores the current size fraction source and species lists to the initially chosen lists. The initial lists were chosen in the initialization phase.

3.3.12 PSOLN

The PSOLN command displays all 31 ridge regression solutions. The display may be directed to the user's terminal or to hardcopy.

The output from this command can be extensive. The program first warns the user by giving the size of the entire solution set. Then the program prompts the user as follows:

ARE YOU SURE YOU WANT TO LOOK AT THESE NUMBERS?

Reply "YES" if still serious. A "NO" will get the prompt ENTER COMMAND.

DO YOU WANT THE SOLUTIONS PRINTED ON THE HARDCOPY? (INSTEAD OF YOUR TERMINAL)

This option allows the user to get the 31 solutions and examine them later. A "YES" response sends the solutions to hardcopy. A "NO" response will display them at the user's terminal.

CAN YOUR TERMINAL DISPLAY A 132 CHARACTER LINE?

Some printer terminals can print a wide 132-character line. Other printer terminals and some CRT's display a 72-character line. On these terminals a 132-character line will "wrap around" and be difficult to read. The program will format the line to either a 132 or a 72-character line, depending on the user response.

3.3.13 PMATRIX

The PMATRIX command displays the source signature matrix, a single source signature, the receptor concentrations, or the source and species codes. The displays may be directed to the user's terminal or to hardcopy.

MATRICES CAN GO TO HARDCOPY

DO YOU WANT THEM DISPLAYED AT YOUR TERMINAL INSTEAD?

A "NO" will send all output to hardcopy. Nothing will be displayed at the user's terminal. A "YES" will result in all output being displayed at the terminal. The command can be re-entered later to redirect output.

WHAT DO YOU WANT TO SEE?

SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS, OR CODES?

OR ARE YOU DONE?

A reply of DONE or a null line will bring the prompt ENTER COMMAND. Otherwise, reply "SOURCE" or "RECEPTOR" or "CODES." The reply "CODES" will display the source and species numbers and input data set codes. The reply "RECEPTOR" will display the receptor concentrations for both fine and coarse size fractions. The reply "SOURCE" will result in the following prompt:

WHAT SIZE FRACTION? (FINE OR COARSE)

Reply FINE for fine fraction source signature data or COARSE for coarse fraction source signature data.

DO YOU WANT TO LOOK AT THE WHOLE MATRIX?

The program will warn the user of its dimensions. A "NO" response will allow the user to select individual source signatures for display. A "YES" response will result in the following query (if output is directed to user's terminal):

CAN YOUR TERMINAL DISPLAY A 132 CHARACTER LINE?

The program will adjust the format to fit either a 72 or 132-character line. See PSOLN command for details.

The source signature matrix is displayed so that the standard error is directly below each matrix item.

If the option to display individual source signatures was selected, the program prompts,

WHICH SOURCE DO YOU WANT?

Key in the source number. The program will display the indicated source data. The prompt will then be reissued. Another source may be displayed, or enter a blank or null line to be returned to the prompt WHAT DO YOU WANT TO SEE?

3.3.14 PINFO

The PINFO command displays the current status of the problem-solving process. This is more useful for CRT users than those with printer terminals.

The command displays the sources and species currently assigned. It also gives the receptor identifier, data, size fraction, and background information. An example of the display appears in Section 4.

3.3.15 AUTOFIT

The AUTOFIT command is an alternative to the SELECT command. The SELECT command selects a single receptor site, date, and size fraction for CMB analysis. In contrast, the AUTOFIT command automatically sequences through a series of sites, dates, and size fractions. The AUTOFIT command is equivalent to a series of SELECT and WRITE commands. However, user responses are minimized by eliminating repetitive keying of commands and responses.

Before using the AUTOFIT command, the user should be familiar with the SELECT command. Like SELECT, the AUTOFIT command invokes the CMB and PDATA commands. It also invokes the WRITE command.

Like the SELECT command, the AUTOFIT command queries the user for site, year, and date. This determines the initial receptor. AUTOFIT does not prompt the user for size fraction because it will do both size fractions. The AUTOFIT sequence next invokes the CMB command and queries the user for the analysis method (ridge regression, effective variance, and intercept options). The method chosen will be used for all receptors and both size fractions in the AUTOFIT series.

The AUTOFIT series begins with the fine fraction of the chosen initial receptor site and date. Then the coarse fraction is analyzed. These analyses are repeated on the next receptor site and date of the Receptor Concentration Data File. The series proceeds in this manner to the end of the file unless terminated by the user.

The user selects the initial receptor site and date according to prompts and replies identical to those under the SELECT command. Then the user chooses the analytical method according to prompts and replies identical to those under the CMB command. There are no further prompts for the rest of the AUTOFIT series except the following (see PDATA command):

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND

This prompt follows the displayed CMB coefficients. If the user enters a null line by pressing RETURN, the program displays the calculated concentrations in addition.

Unlike SELECT, entering a "C" under the AUTOFIT command will not bring up the prompt "ENTER COMMAND." Instead, the program proceeds to the

next analysis, which it also does after displaying the calculated concentrations. The AUTOFIT sequence can be terminated at this point by keying in "STOP." The program then prompts "ENTER COMMAND."

If the user determines that he has mistakenly terminated the AUTOFIT series, it is not necessary to start over. The command RESUME may be entered immediately after the stop response to continue the AUTOFIT series.

3.3.16 RESUME

The RESUME command should only be used in conjunction with the AUTOFIT command. If the AUTOFIT sequence has been mistakenly terminated by a STOP response, the RESUME command will continue the autofit sequence.

3.3.17 BACKOUT

The BACKOUT command allows the user to remove the effect of background concentration from receptor concentration data. Subsequent CMB analyses reflect the background adjustment. The BACKIN command reverses the BACKOUT effects.

The BACKOUT command acts on the site/date receptor of the latest SELECT (or AUTOFIT) command. The queries and replies for the BACKOUT command are similar to those of the SELECT command:

ENTER BACKGROUND CMB SITE CODE: XXXXXXXXXXXXX

The user should enter the CMB site code for the site chosen to represent background concentration. Subsequent queries identical with those of the SELECT command ask for year and date. The user is not queried for size fraction since both sizes are adjusted.

3.3.18 BACKIN

The BACKIN command removes the background adjustment to receptor concentrations applied by BACKOUT. The user should be aware that some roundoff error may occur so that the BACKIN reversal of BACKOUT may not be perfect.

3.3.19 PCOMP

The PCOMP command computes and prints the average contributions of each source from a series of CMB analyses. The PCOMP command should follow an AUTOFIT command or a series of SELECT-WRITE commands emulating an AUTOFIT series.

A typical set of receptor concentration data could include a series of sampling dates at one receptor station or a group of receptors in a target area. The user would naturally want to compute the "average" CMB results in these cases. This is the purpose of PCOMP.

For PCOMP to work properly it must be preceded by a series of SELECT and WRITE commands for both fine and coarse fractions of each desired receptor concentration data set. The AUTOFIT does this automatically. Careful use of the SELECT and WRITE commands achieve the same end. However, whenever possible, the AUTOFIT command should be used to avoid errors.

The PCOMP command computes the average contribution from all complete CMB analyses following the previous PCOMP command or the initialization phase, whichever is later. The complete CMB analyses are those that included both fine and coarse analyses each followed by the WRITE command.

The output includes the labeled CMB coefficients from the averaged analyses, the averages according to sources, and the standard deviations. For each source, the mean and standard deviation are computed directly

from the solutions for the different cases. A "solution" here is the calculated contribution to the ambient aerosol of a particular source. The means and standard deviations are not adjusted to account for the correlated error effect discussed in Section 2.

The PCOMP command gives one prompt to the user:

```
OUTPUT WILL GO TO HARDCOPY
DO YOU WANT IT DISPLAYED AT YOUR TERMINAL INSTEAD?
```

The user response "NO" will result in the output being written on the hardcopy. A "YES" brings the display to the user's terminal.

3.3.20 EXIT

The EXIT command terminates the interactive session. The user is returned to the time sharing system.

3.4 Detailed Formats of Data Files

The various input data files must be coded according to the specific formats presented here. The formats are presented as card images. However, the data should be on files accessible in interactive mode. For the receptor concentrations the data must be on a unit that responds to a FORTRAN REWIND. The other input data files are read only once.

Each data file line format is presented. Except for the receptor concentration data file, each data file includes only one card type. Since the CMB program is written in FORTRAN, the FORTRAN format of each item is given for the convenience of the user in determining acceptable entries.

In the following, the FORTRAN formats A, I, and F are referred to. The A format is used to read alphanumeric information. The integer

following the A, e.g., the 8 in A8, gives the width of the field. The I format is used to read integers. For example, if the format is I4, the integer must be right-justified in a 4-character-wide field. Decimal points are not used with I format. The F format is used to read "floating-point," or arbitrary real numbers. The format F8.6 indicates that the field is 8 characters wide, and the rightmost 6 characters occur after the decimal point. For example, the number 12345678 would be read as 12.345678. More commonly, however, the decimal point is supplied. In this case the number can appear anywhere in the field.

All of the following numbers would be read as 12.3 if format F8.6 was used:

```

12.3____
__12.3__
____12.3

```

where the underscores indicate blanks.

Source Names and Codes		
<u>Column</u>	<u>Format</u>	<u>Contents</u>
1-2	I2	Source code.
3-4	-	Skipped.
5-12	A8	Source Name.
13-80	-	Skipped. May contain user comment.

Species Names and Codes		
<u>Column</u>	<u>Format</u>	<u>Contents</u>
1-2	I2	Species Code.
3-4	-	Skipped.
5-12	A8	Species Name.
13-80	-	Skipped. May contain user comment.

The fine and coarse fraction source signature matrices use the same line format.

Source Signature Matrix		
Column	Format	Contents
1-2	I2	Source Code.
3-4	-	Skipped.
5-6	I2	Species Code.
7-8	-	Skipped.
9-16	F8.6	Fraction of Source for Species.
17-18	-	Skipped
19-26	F8.6	Standard Error of Fraction.
27-80	-	Skipped. May contain user comment.

A species code of '01' should not be used. Species code one is reserved for total aerosol. The program automatically generates the source signature vector for total aerosol.

The Receptor Concentration Data Set includes two card types. The card type '03' identifies the receptor. There is only one card type '03' per sampling date for each receptor location. The card type '30' gives the actual concentration data. There is a card type '30' for each species. The card type '30' lines follow directly after the corresponding card type '03.'

The concentration data may consist of fine and coarse fractions or of the fine fraction and total. This data type is indicated on the card type '03.'

Species code '01' is reserved for total aerosol. The total aerosol data are used in selecting the "best" ridge regression solution.

Receptor Concentration Data--Card Type 03 (Identification)		
Column	Format	Contents
1-2	I2	'03'--card type.
3	-	Skipped.
4-15	3A4	Receptor identification.
16	-	Skipped.
17-18	A2	Year.
19-22	A4	Month and Day (MMDD).
23	-	Skipped.
24-25	I2	Duration of Sample (hours).
26	-	Skipped.
27-28	I2	Start hour of Sample.
29-32	-	Skipped.
33-34	I2	Data Type. '12'--Fine and Coarse '13'--Fine and Total
35-80	-	Must be blank.

Receptor Concentration Data--Card Type 30		
Column	Format	Contents
1-2	I2	'30'--card type.
3	-	Skipped.
4-15	3A4	Receptor identification.
16	-	Skipped.
17-18	A2	Year.
19-22	A4	Month and Day (MMDD).
23	-	Skipped.
24-25	I2	Duration of Sample (hours).
26	-	Skipped.
27-28	I2	Start hour of Sample.
29-32	-	Skipped.
33-34	I2	Species Code.
35-36	-	Skipped.
37-45	F9.4	Fine Fraction Concentration.
46-47	-	Skipped.
48-56	F9.4	Standard Error of Fine Fraction.
57-58	-	Skipped.
59-67	F9.4	Coarse Fraction/Total Concentration.
68-69	-	Skipped.
70-78	F9.4	Standard Error of Coarse Fraction/Total.
79-80	-	Skipped.

The user followup data file is produced by the program and is not coded by the user. The format of the user followup data file is documented here for those who wish to make use of it.

The user followup data file includes three card types. Card types '03' and '30' are the same as Receptor Concentration Data Set card types '03' and '30'. Card type '40' gives the species concentration contributed by each source.

Recall that species 01 is the aerosol mass concentration for the size fraction being considered. The card type '40' entries for species 01 give the total aerosol contributions for their size fraction for the different sources.

Card types '03' and '30' are written whenever a receptor site and date are selected by the SELECT or AUTOFIT commands. Card type '40' is written by the WRITE command when both fine and coarse size fractions have been analyzed in succession.

User Followup Data--Card Type 40		
<u>Column</u>	<u>Format</u>	<u>Contents</u>
1-2	I2	'40'--card type.
3	-	Skipped.
4-15	3A4	Receptor identification.
16	-	Skipped.
17-18	A2	Year.
19-22	A4	Month and Day (MMDD).
23	-	Skipped.
24-25	I2	Duration of Sample (hours).
26	-	Skipped.
27-28	I2	Start hour of Sample.
29	-	Skipped.
30-31	I2	Source Code.
32	-	Skipped.

User Followup Data--Card Type 40 (continued)		
<u>Column</u>	<u>Format</u>	<u>Contents</u>
33-34	I2	Species Code.
35-36	-	Skipped.
37-45	F9.4	Fine Fraction Contribution ($\mu\text{g}/\text{m}^3$)
46-47	-	Skipped.
48-56	F9.4	Uncertainty of Fine Fraction.
57-58	-	Skipped.
59-67	F9.4	Coarse Fraction Contribution.
68-69	-	Skipped.
70-78	F9.4	Uncertainty of Coarse Fraction.
79-80	-	Skipped.

3.5 Command Reference Summary

This section gives a short description of the purpose and results of each command. This summary is intended to serve as a quick and ready reference for the user. Commands must be spelled out in full. However, a response to a query may be abbreviated by the first letter unless a numerical value or alphanumeric code is requested. Command details are given in Section 3.2.

HELP--This command lists all the commands with a brief statement of the purpose of each one.

SELECT--This command is used to select the receptor data set for the current CMB analysis. SELECT also automatically invokes CMB and PDATA. The user is prompted for the site, year, date and size fraction.

CMB--This command is used to determine the specific method options and to perform the CMB analysis. CMB also automatically invokes PDATA. Method options with CMB are ridge regression/least squares, effective variance method/no effective variances, and fitted model intercept/zero intercept. These options may be exercised in any combination.

PDATA--This command displays the current analysis solution at the user's terminal. The output consists of the solution coefficients and standard errors. The least squares coefficients, standard errors, and variance inflation factors are also displayed. Optionally, the receptor data and predicted values may be displayed for all species.

WRITE--This command writes results to hardcopy files. The WRITE command should follow the SELECT or CMB commands.

AE--This command is used to add species to the current fitting set. The program prompts the user for species to add.

DE--This command is used to delete species from the current fitting set. The program prompts the user for species to delete.

AS--This command is used to add sources to the current fitting set. The program prompts the user for sources to add.

DS--This command is used to delete sources from the current fitting set. The program prompts the user for sources to delete.

AUTOFIT--This command is used to perform automatically CMB analyses on a series of sites or dates (for both fine and coarse fractions). The AUTOFIT command saves time and prevents errors by eliminating repetitive entries. The AUTOFIT command is equivalent to a series of SELECT (CMB, PDATA) and WRITE commands.

RESUME--This command is used in conjunction with AUTOFIT to resume the autofit sequence.

BACKOUT--This command is used to remove the effect of background concentrations from receptor data. This command should be invoked after SELECT. The program prompts the user for site, year and date.

BACKIN--This command is used to cancel the effect of the BACKOUT command.

PMATRIX--This command is used to display the source signature matrix, the receptor data, species code list, and source code list. The program prompts the user for the items to display. Optionally, the output may go to the user's terminal or to hardcopy.

PSOLN--This command is used to display all ridge solutions, not merely the "best" one. Optionally, the output may go to the user's terminal or to hardcopy.

PINFO--This command displays the current problem status giving site, date, size, and background information. It is primarily useful to users of CRT terminals.

PCOMP--This command is used to compute and print the averages and standard deviations of a series of CMB analyses. Optionally, the output may go to the user's terminal or to hardcopy.

EXIT--This command terminates the CMB program processing.

3.6. Computer System Considerations

Certain tasks relevant to using the CMB program are contingent on the conventions of the particular computer being used. These include compilation and subprogram linkage, file access, and program execution. This section gives information pertinent to computer dependency. The emphasis of this information is oriented towards the EXEC 8 system of the Univac 1100 series, which was used in the program development. The requirements of IBM TSO are given a shorter discussion. The command names and syntax vary, but the tasks that must be performed are similar regardless of computer systems.

The physical characteristics of the eleven files accessed by the CMB program are as follows:

<u>FORTTRAN</u> <u>Unit #</u>	<u>Input/Output</u>	<u>Record or Line Length</u>
2	Input	80
3	Input	80
5	Input	72 (Terminal)
6	Output	72 to 132 (Terminal)
7	Input	80
8	Input	80
9	Output	121 (Print File)
10	Input/Output	80 (Scratch Data File)
11	Output	133 (Print File)
12	Output	80
13	Input	80

The CMB program consists of a main program and five subprograms. All programs are written in FORTRAN. These programs are the following:

<u>Program</u>	<u>Purpose</u>
MAIN	Initialization and command sequence
FETCH	Read receptor concentration data
CMBR	Perform CMB analysis
PERC	Compute percentages and variances
COARS	Compute coarse fraction and variances
INV1	Matrix inversion

The program MAIN calls FETCH, CMBR, and PERC. FETCH calls COARS; CMBR calls INV1.

3.6.1 Univac System Conventions

This section describes one approach to using the CMB program on a Univac 1100 series computer. Other approaches are feasible. If the directions given here are followed, the CMB program can be invoked by a statement like the following:

```
@ADD CMB-RADPRG.HCS-FILE
```

Similarly, the hardcopy files may be printed by a statement like the following:

```
@ADD CMB-RADPRG.HCS-PRT
```

The following steps prepare the source code for execution. These steps need be performed only once if the result is saved.

```
@FTN,U CMB-RADPRG.MAIN,CMB-RADPRG.MAIN
@FTN,U CMB-RADPRG.FETCH,CMB-RADPRG.FETCH
@FTN,U CMB-RADPRG.CMBR,CMB-RADPRG.CMBR
@FTN,U CMB-RADPRG.PERC,CMB-RADPRG.PERC
@FTN,U CMB-RADPRG.COARS,CMB-RADPRG.COARS
@FTN,U CMB-RADPRG.INV1,CMB-RADPRG.INV1
@MAP,I CMB-RADPRG.MAP,CMB-RADPRG.CMB
IN CMB-RADPRG.MAIN,.CMBR,.COARS,.FETCH,.PERC,.INV1
END
```

The input data files must contain the data for the analyses. If the data are punched on cards, the cards may be loaded to the files using the @ELT command, as in the following example:

```
@ELT CMB-RADPRG.HCS-SORF
  --DATA CARDS FOR FINE SOURCE SIGNATURE--
@ELT CMB-RADPRG.HCS-SORC
  --DATA CARDS FOR COARSE SOURCE SIGNATURE--
@ELT CMB-RADPRG.HCS-DATA
  --DATA CARDS FOR RECEPTOR CONCENTRATION DATA--
@ELT CMB-RADPRG.HCS-PONM
  --DATA CARDS FOR SPECIES NAMES & CODES--
@ELT CMB-RADPRG.HCS-SONM
  --DATA CARDS FOR SOURCE NAMES & CODES--
```

Alternatively, the data may be entered directly onto the file in an interactive session using the editor:

```
@ED,I CMB-RADPRG.HCS-SORF
--DATA LINES FOR FINE SOURCE SIGNATURE--
ETC.
```

The following command sequence will define the files and begin execution of the CMB program. For convenience, these commands are best placed on a file element (using the editor) and brought into the runstream with an @ADD command. The approach given here assigns temporary SDF files, copies the permanent data onto the temporary files, sets up the FORTRAN unit numbers, and executes the CMB program.

```
@ASG,A CMB-RADPRG.
@FREE CMB-RADPRG.
@ASG,T TEMP.
@ASG,T MAGSTO.
@ASG,T SUMMRY.
@ASG,T CMBOUT.
@ASG,T HCS-PONM.
@ASG,T HCS-SORC.
@ASG,T HCS-SORF.
@ASG,T HCS-DATA.
@ASG,T HCS-SONM.
@COPY,I CMB-RADPRG.HCS-PONM,HCS-PONM.
@COPY,I CMB-RADPRG.HCS-SORC,HCS-SORC.
@COPY,I CMB-RADPRG.HCS-SORF,HCS-SORF.
@COPY,I CMB-RADPRG.HCS-DATA,HCS-DATA.
@COPY,I CMB-RADPRG.HCS-SONM,HCS-SONM.
@USE 2.,HCS-SONM.
@USE 3.,HCS-PONM.
@USE 7.,HCS-SORF.
```

```

@USE 8.,HCS-SORC.
@USE 9.,SUMMRY.
@USE 10.,TEMP.
@USE 11.,CMBOUT.
@USE 12.,MAGSTO.
@USE 13.,HCS-DATA.
@XQT CMB-RADPRG.CMB

```

These lines would be the contents of the file CMB-RADPRG.HCS-FILE used in the @ADD statement given at the beginning of this subsection.

These control statements or the equivalent @ADD statement begin the execution of the CMB program. The program proceeds as described in Sections 3.2 and 3.3. After the user has issued the EXIT command to the CMB program, control is returned to the system.

If the user's terminal is a printer terminal with 132 character print line width, then it can be used to print the hardcopy files and the user followup data file:

```

@HDG,P *** CMB MODEL : OUTPUT 'SUMMRY' DATA FILE ***
@ED,R SUMMRY.
P!
EXIT
@HDG,P *** CMB MODEL : OUTPUT 'CMBOUT' DATA FILE ***
@ED,R CMBOUT.
P!
EXIT
@HDG,P *** CMB MODEL : OUTPUT 'USER FOLLOWUP' DATA FILE ***
@ED,R MAGSTO.
P!
EXIT

```

These lines would be the content of the file CMB-RADPRG.HCS-FILE used in the @ADD statement given at the beginning of this subsection.

Alternatively, the results may be saved permanently for later printing on the system printer:

```
@COPY,I CMBOUT.,CMB-RADPRG.CMBOUT
@COPY,I SUMMRY.,CMB-RADPRG.SUMMRY
@COPY,I MAGSTO.,CMB-RADPRG.MAGSTO
```

3.6.2 IBM TSO System Considerations

The CMB program was developed on a Univac 1100 series computer. Nevertheless, every conscious effort was made to render the code compatible with IBM FORTRAN.

This section will briefly discuss the IBM TSO conventions needed to execute the CMB program.

The CMB programs can be compiled using the TSO FORT command or one of the FORTRAN batch compilers. The programs can be linked into a load module using the TSO LINK command or the batch linkage editor.

The input data files may be loaded from cards using the IBM utility IEBGENER. Alternatively, the lines may be entered directly using the TSO EDIT command.

The data files may be assigned FORTRAN unit numbers using the TSO ALLOCATE command, as in the following example:

```
ALLOC DA(CMB.HCS.PONM.DATA) F(FT03F001)
```

The program can be executed using the TSO CALL command, as in the following example:

```
CALL    CMB.PDS,LOAD(CMB)
```

The ALLOCATE commands and the CALL command can be organized into a CLIST so that a single EXEC command will begin the CMB program execution.

The hardcopy prints may be displayed at the user's terminal using the TSO EDIT LIST command or sent to the system printer using the IBM utility PRTPCH.

SECTION 4

EXAMPLE RUN

4.1 Introduction

This section presents an example interactive session using the CMB program. This run of the CMB program exercises all of the commands. The purpose of this run is to illustrate the use of each command, and, as a result, it does not necessarily follow the course that an actual analysis might take. Moreover, the course of an actual analysis can vary significantly, depending on the nature and size of the ambient receptor data set and the objectives to be achieved by the analyses.

The example runs were executed on EPA's Univac 1100 series computer. The program was invoked with the command

```
@ADD CMB-RADPRG.HCS-FILE
```

as described in Section 3.6. The user's entries are preceded in the session by the symbol ">".

4.2 Illustration of Commands

```
WOULD YOU LIKE TO LOOK AT THE SOURCE AND SPECIES LISTS?  
TYPE YES OR NO.
```

The user replies "YES" so that he will get a list of the source and species numbers to refer to in the rest of the interactive session.

>YES

SOURCE SIGNATURE MATRICES ARE CODED AS FOLLOWS

SOURCES:

SOURCE #	SOURCE NAME
----------	-------------

1	SOIL
2	RD DUST
3	SEA SALT
4	SLSH BRN
5	AUTO CAT
6	AUTO
7	JET AIR
8	RES OIL
9	DIST OIL
10	RES GAS
11	COAL
12	KRAFT RB
13	ELARCFRN
14	FERRKNFR
15	CAL GYP
16	CEMENT
17	PET FCC
18	LSKILN
19	SEC SO4

SPECIES:

SPECIES #	SPECIES NAME
-----------	--------------

1	TOTAL
2	AL
3	AS
4	BA
5	BR
6	CA
7	CD
8	CL
9	CO
10	CR
11	CU
12	FE
13	HG
14	K
15	MN
16	NI
17	P
18	PB
19	SO4
20	SB
21	SI
22	SN
23	SR
24	TI

25	V
26	ZN
27	C
28	NA
29	NO3
30	RB
31	SE

Next, the user selects the sources using the source numbers in the above list. The user keys a "RETURN" or null line for "INITIAL SOURCE 15" to indicate that he has entered all of the desired sources. The program displays a list of the selected sources with their source numbers for the user's verification.

PLEASE INPUT INITIAL FITTING INFORMATION

```

INITIAL SOURCE  1: XX
>1
INITIAL SOURCE  2: XX
>2
INITIAL SOURCE  3: XX
>3
INITIAL SOURCE  4: XX
>5
INITIAL SOURCE  5: XX
>6
INITIAL SOURCE  6: XX
>7
INITIAL SOURCE  7: XX
>9
INITIAL SOURCE  8: XX
>10
INITIAL SOURCE  9: XX
>11
INITIAL SOURCE 10: XX
>12
INITIAL SOURCE 11: XX
>13
INITIAL SOURCE 12: XX
>14

```

```

INITIAL SOURCE 13: XX
>16
INITIAL SOURCE 14: XX
>17
INITIAL SOURCE 15: XX
>
INITIAL SOURCES
  1 SOIL
  2 RD DUST
  3 SEA SALT
  5 AUTO CAT
  6 AUTO
  7 JET AIR
  9 DIST OIL
 10 RES GAS
 11 COAL
 12 KRAFT RB
 13 ELARCFRN
 14 FERRMFR
 16 CEMENT
 17 PET FCC

```

Next the user selects the species. This can be done individually as above with the sources. However, the user wants to enter "all" of the species. He keys a "-1" for "INITIAL SPECIES 1" and the first 21 (maximum allowable) species are selected. The program displays a list of them for the user's verification.

```

PLEASE INPUT SPECIES
INITIAL SPECIES 1: XX
>-1
INITIAL SPECIES
  1 TOTAL
  2 AL
  3 AS
  4 BA
  5 BR
  6 CA
  7 CD
  8 CL
  9 CO

```

10	CR
11	CU
12	FE
13	HG
14	K
15	MN
16	NI
17	P
18	PB
19	SO4
20	SB
21	SI

Next the program asks the user if the selected sources and species are correct. The user is satisfied with his choices (for the time being) and replies "YES." Then the program notes that the current size fraction is fine (rather than coarse). The session now enters the command phase.

```
ARE INITIAL SOURCES AND SPECIES CORRECT?
>YES
THE "HELP" COMMAND LISTS COMMANDS
SIZE IS FINE
ENTER COMMAND
```

The user decides to give the HELP command to get a list of the commands and their uses.

```
HELP
HELP-LISTS THESE COMMANDS

---- DATA ACCESS AND SEQUENCING ----
AUTOFIT-SEQUENCES AUTOMATICALLY TO NEXT DATA SET
RESUME-RESUME AUTOFIT
SELECT-SELECT DATA SET FOR CMB
SIZE-CHANGE SIZE FRACTION
EXIT-CLOSE FILES AND LEAVE
```

---- CMB OPERATIONS ----
AE-ADD A SPECIES TO THE FIT
DE-DELETE A SPECIES FROM THE FIT
AS-ADD A SOURCE TO THE FIT
DS-DELETE A SOURCE FROM THE FIT
CMB-PERFORM CMB: OPTIONS ARE RIDGE & EFFECTIVE VARIANCE

---- SCREEN DISPLAY ----
PINFO-PRINT CURRENT STATUS ON SCREEN
PDATA-PRINT CURRENT CMB RESULTS ON SCREEN
PMATRIX-PRINT SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS,
OR SOURCE AND SPECIES CODE LISTS
PSOLN-PRINT ALL RIDGE SOLUTIONS
PCOMP-PRINT COMPUTED AVERAGES OF CMB SERIES

---- DATA STORAGE ----
WRITE-WRITE PRESENT CMB RESULTS TO FULL PRINTOUT,
SUMMARY,AND USER FOLLOWUP STORAGE FILES

---- BACKGROUND SITE OPERATIONS ----
BACKOUT-SELECT AND SUBTRACT A BACKGROUND DATA SET
BACKIN-ELIMINATE CURRENT BACKGROUND SUBTRACTION

SELECT SHOULD NORMALLY BE THE FIRST COMMAND
ENTER COMMAND

The SELECT command will bring in receptor concentration data.

>SELECT
ENTER DESIRED CMB SITE CODE: XXXXXXXXXXXX

If the user does not know how the receptor sites are coded, he can reply with a question mark or any other incorrect response. Then the program will list the sites for him:

?
ENTER YEAR: YY
?
ENTER DATE: MMDD
?
INPUT DESIRED SIZE FRACTION:(FINE OR COARSE)

```

>
DATA SEARCH BEGUN FOR
  SITE: ?           YEAR:      DATE:

      SITE: URBAN CORE   YEAR: 81  DATE: 0229   FC
      SITE: BACKGROUND  YEAR: 81  DATE: 0229   FC
DATA SET NOT FOUND FOR
  SITE: ?           YEAR:      DATE:
USE ONE OF THOSE LISTED ABOVE
ENTER COMMAND

```

Now the user knows what receptor site data are available. He gives the SELECT command again, choosing the Urban Core site. The sites and dates available depend on the data in the Receptor Concentration Data File described in Section 3. The data available for this interactive session are given in Appendix C.

```

>SELECT
ENTER DESIRED CMB SITE CODE: XXXXXXXXXXXX
>URBAN CORE
ENTER YEAR: YY
>81
ENTER DATE: MMDD
>0229
INPUT DESIRED SIZE FRACTION: (FINE OR COARSE)
>FINE
DATA SEARCH BEGUN FOR
  SITE: URBAN CORE   YEAR: 81  DATE: 0229

      SITE: URBAN CORE   YEAR: 81  DATE: 0229   FC

```

The program now automatically moves into the CMB command.

```

DO YOU WANT RIDGE SOLUTIONS?
>YES
CMB WILL SELECT THE BEST RIDGE SOLUTION
DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?
>NO
IN THE SELECTION OF THE BEST RIDGE SOLUTION,
WHAT WEIGHT DO YOU WANT? (DEFAULT=1.0)
>
WEIGHT IS          1.000000000
DO YOU WANT TO USE EFFECTIVE VARIANCES?
>NO
DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?
>YES

```

The user selects the method options by replying appropriately to the questions asked. The summary of the ridge solutions is illustrated later in this session. The default weight is selected by keying a RETURN or null line. Keying in "1.0" would have the same effect. Note that if a weight is given, the decimal point must be included.

The program now automatically enters the command PDATA.

```

CMB SITE: URBAN CORE      YEAR: 81    DATE: 0229    FRACTION: FINE
SAMPLE DURATION: 12 WITH START HOUR: 7  BACKGROUND: NO  EFF VAR: NO
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .8991  RIDGE K= .050      R-SQUARE: .9139
---SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .004+-      .005      .004+-      .008
1 SOIL            .448+-      1.089      -6.760+-      53.326 1383.677
2 RD DUST         .011+-      .858       .878+-       6.047  86.913
3 SEA SALT        -.313+-      .138      -.572+-       .869 128.630
5 AUTO CAT        9.566+-      9.073     -6.683+-      80.143 113.999
6 AUTO            4.013+-      .957       4.790+-       1.135  3.290
7 JET AIR         3.520+-      44.126     3.542+-      58.707  1.941
9 DIST OIL        .944+-      5.510       7.215+-      18.067 34.277
10 RES GAS        .295+-      2.361     12.645+-      86.973 1090.330
11 COAL           1.931+-      1.899       2.149+-      16.839 139.242
12 KRAFT RB       -.095+-      2.467       .912+-      24.370 219.996
13 ELARCFRN       .028+-      .190      -.033+-       3.765 553.312
14 FERRMFR        .085+-      .145       .126+-       1.834 186.655
16 CEMENT         6.487+-      2.443       7.071+-      27.846 237.782
17 PET FCC        7.900+-      6.591       9.716+-      72.098 198.829
TOTAL:           34.824+-      48.266     35.000+-      50.671
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
35.00000+-      7.000/ 75.00000+-      7.000/ 110.00000+-      9.899

```

This table presents the fitted coefficients and their standard errors for each source. Two sets of coefficients are given: the solution on the left is the "best" ridge solution ($k = 0.050$) and the solution on the right is the weighted least squares solution ($k = 0.0$).

The solutions consist of coefficient estimates with standard errors for each source. Variance inflation factors are given at the far right. At the bottom the calculated total aerosol is given for each solution. The measured total aerosol is also given for each size fraction.

Due to the complexity of the set of sources used and possibly also to uncertainties in the source signatures, both solutions contain large random errors for some sources. The large variance inflation factors for some sources indicate that strong multicollinearities exist. Notice, however, that the ridge solution has greatly reduced standard errors for the sources with large variance inflation factors. Also, the ridge solution has no significant negatives, although the weighted least squares solution has negatives with large magnitudes. This is typical in problems affected by multicollinearity.

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND

The user can now proceed to a new command by entering a "C." However, the user wants to examine the calculated concentrations. He presses the return key to get this table:

		-----MEAS-----		-----CALC-----		-----RATIO-----		
1	TOTAL	*	35.000+- 7.000	34.824+-48.266	.99+- 1.39	TOT		
2	AL	*	.088+- .062	.033+- .004	.38+- .27	AL		
3	AS	*	.036+- .007	.004+- .000	.12+- .02	AS		
4	BA	*	.149+- .014	.005+- .000	.03+- .00	BA		
5	BR	*	.344+- .017	.334+- .082	.97+- .24	BR		
6	CA	*	.441+- .023	.441+- .082	1.00+- .19	CA		
7	CD	*	.004+- .002	.006+- .000	1.55+- .78	CD		
8	CL	*	.051+- .007	.060+- .069	1.17+- 1.37	CL		
9	CO	*	.003+- .002	.004+- .000	1.50+- 1.00	CO		
10	CR	*	< .004	.005+- .000	2.58+- 5.16	CR		
11	CU	*	.013+- .002	.009+- .001	.71+- .12	CU		
12	FE	*	.208+- .011	.203+- .029	.97+- .15	FE		
13	H6	*	< .003	.004+- .000	.00+- .00	H6		
14	K	*	.165+- .009	.148+- .033	.90+- .20	K		
15	MN	*	.022+- .004	.023+- .004	1.06+- .26	MN		
16	NI	*	.006+- .001	.006+- .000	1.04+- .18	NI		
17	P	*	.119+- .017	.004+- .000	.04+- .01	P		
18	PB	*	1.422+- .068	.870+- .212	.61+- .15	PB		
19	SO4	*	13.130+- .681	13.027+- 1.832	.99+- .15	SO4		
20	SB	*	.003+- .002	.005+- .000	1.68+- 1.12	SB		
21	SI	*	.277+- .031	.305+- .046	1.10+- .21	SI		
22	SN		< .002	.020+- .004	20.40+-40.99	SN		
23	SR		.003+- .001	.005+- .000	1.54+- .51	SR		
24	TI		< .014	.008+- .001	1.09+- 2.18	TI		
25	V		< .008	.005+- .000	2.29+- 9.15	V		
26	ZN		.042+- .003	.046+- .008	1.08+- .21	ZN		
27	C	M	< .001	10.518+- 1.383	.00+- .00	C		
28	NA	M	< .001	-.094+- .024	.00+- .00	NA		
29	NO3	M	< .001	.019+- .003	.00+- .00	NO3		
30	RB	M	< .001	.004+- .000	.00+- .00	RB		
31	SE	M	< .001	.004+- .000	.00+- .00	SE		

ENTER COMMAND

For each species available the table above gives the measured concentration, the calculated concentration, and the ratio of the calculated to the measured concentration. Each quantity is accompanied by its standard error.

Those species that were included in the fitting process are marked with an asterisk (*). Those species that are marked with an "M" do not have receptor concentration data.

The user has the option to change the selection of sources and species and reperform the analysis. The effect of deleting undetected species Cr and Hg (10 and 13) and adding the detected but unused species Sr and Zn (23 and 26) could be investigated. In general, however, species which serve as key tracers for important sources should be included even if those species have small ambient concentrations. A tracer could be a species which constituted a small percentage of the aerosols from a given source but which was virtually unique to that source. Sources with negative coefficients are candidates for removal. Also, sources with standard errors many times larger than their coefficients are potential deletions. The indication is that the contribution of such sources is zero within random variability. The large SO_4 measured concentration indicates that sulfate sources are important. The secondary sulfate source (19) is a potential addition.

Upon examining his first trial the user determines that he wishes to change some of the fitting species and sources. He uses the DE command to delete species, the AE command to add species, the DS command to delete sources, and the AS command to add sources. In each case, the user terminates the command with a RETURN.

```
>DE
SIZE IS FINE
INPUT CODE OF DELETED SPECIES
>10
INPUT CODE OF DELETED SPECIES
>13
INPUT CODE OF DELETED SPECIES
>
ENTER COMMAND
/AE
SIZE IS FINE
INPUT CODE OF ADDED SPECIES
/23
INPUT CODE OF ADDED SPECIES
/26
```

```

INPUT CODE OF ADDED SPECIES
>
ENTER COMMAND
>DS
SIZE IS FINE
INPUT CODE OF DELETED SOURCE
>12
INPUT CODE OF DELETED SOURCE
??
INPUT CODE OF DELETED SOURCE
>
ENTER COMMAND
>AS
SIZE IS FINE
INPUT CODE OF ADDED SOURCE
>19
INPUT CODE OF ADDED SOURCE
>
ENTER COMMAND

```

Now the user is ready to rerun the CMB analysis. It is not necessary to use SELECT again since the data have been already brought in for the desired site. Therefore, the user gives the CMB command.

```

CMB
DO YOU WANT RIDGE SOLUTIONS?
>YES
CMB WILL SELECT THE BEST RIDGE SOLUTION
DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?
>NO
IN THE SELECTION OF THE BEST RIDGE SOLUTION,
WHAT WEIGHT DO YOU WANT? (DEFAULT=1.0)
>
WEIGHT IS 1.000000000
DO YOU WANT TO USE EFFECTIVE VARIANCES?
>NO
DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?
>YES

```

```

CMB SITE: URBAN CORE      YEAR: 81    DATE: 0229    FRACTION: FINE
SAMPLE DURATION: 12 WITH START HOUR: 7 BACKGROUND: NO EFF VAR: NO
-----RIDGE REGRESSION-----
R-SQUARE: .9179    RIDGE K= .010
-----SOURCE-----UG/M3-----
INTERCEPT      .004+-    .004
1 SOIL            -.509+-    3.092
2 RD DUST         -.024+-    .923
3 SEA SALT        -.446+-    .171
5 AUTO CAT       7.377+-    20.436
6 AUTO           4.635+-    .941
9 DIST OIL       3.596+-    6.614
10 RES GAS       1.015+-    5.311
11 COAL          1.771+-    1.348
13 ELARCFRN      .076+-    .454
14 FERRMFR       .061+-    .250
16 CEMENT        7.403+-    2.919
17 PET FCC       8.221+-    12.252
19 SEC SO4       -.187+-    11.012
TOTAL:          32.991+-    15.162
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
35.00000+-    7.000/ 75.00000+-    7.000/ 110.00000+-    9.899
-----WEIGHTED LEAST SQUARES-----
R-SQUARE: .9200
-----UG/M3-----VIF-----
INTERCEPT      .005+-    .006
-8.858+-    27.313    432.869
.891+-    3.239    29.638
-.533+-    .265    14.234
-2.525+-    58.257    79.398
4.800+-    .975    2.881
6.549+-    10.723    14.366
15.427+-    49.140    413.108
2.192+-    2.462    9.374
.048+-    1.249    71.640
.083+-    .612    24.698
7.999+-    4.322    6.798
9.410+-    41.216    77.121
-3.353+-    49.346    173.618
TOTAL:          32.136+-    50.953

```

```

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>C
ENTER COMMAND

```

This time the user gives a "C" and no receptor concentrations are displayed.

The user is now ready to look at the coarse fraction. The SIZE command switches the current size to coarse. Then the user adjusts his selection of sources. The species and sources for the coarse size fraction were not affected by the adjustments made for the fine fraction earlier.

```

SIZE
SIZE IS COARSE
ENTER COMMAND
>DE
SIZE IS COARSE
INPUT CODE OF DELETED SPECIES
>3
INPUT CODE OF DELETED SPECIES
>7
INPUT CODE OF DELETED SPECIES
>13
INPUT CODE OF DELETED SPECIES
>16
INPUT CODE OF DELETED SPECIES
>19
INPUT CODE OF DELETED SPECIES
>20
INPUT CODE OF DELETED SPECIES
>
ENTER COMMAND
>AE
SIZE IS COARSE
INPUT CODE OF ADDED SPECIES
>23
INPUT CODE OF ADDED SPECIES
>24
INPUT CODE OF ADDED SPECIES
>26
INPUT CODE OF ADDED SPECIES
>
ENTER COMMAND
>DS
SIZE IS COARSE
INPUT CODE OF DELETED SOURCE
>7
INPUT CODE OF DELETED SOURCE
>9
INPUT CODE OF DELETED SOURCE
>10
INPUT CODE OF DELETED SOURCE
>13
INPUT CODE OF DELETED SOURCE
>14
INPUT CODE OF DELETED SOURCE
>17
INPUT CODE OF DELETED SOURCE
>
ENTER COMMAND

```

Now the user asks for a CMB analysis of the coarse fraction.

```

>CMB
DO YOU WANT RIDGE SOLUTIONS?
>SAME

CMB SITE: URBAN CORE      YEAR: 81    DATE: 0229    FRACTION: COARSE
SAMPLE DURATION: 12 WITH START HOUR: 7  BACKGROUND: NO  EFF VAR: NO
-----RIDGE REGRESSION-----    -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .6151    RIDGE K= .800    R-SQUARE: .7702
-----SOURCE-----UG/M3-----    -----UG/M3-----VIF-----
INTERCEPT    .011+-    .005    .023+-    .010
1 SOIL    36.445+-    18.752    77.894+-    81.347    6.178
2 RD DUST    13.578+-    6.185    18.281+-    13.310    2.184
3 SEA SALT    .177+-    .491    .365+-    .771    1.223
5 AUTO CAT    10.339+-    13.655    -51.096+-    63.596    6.754
6 AUTO    .722+-    .275    1.180+-    .395    1.054
11 COAL    4.532+-    3.137    11.906+-    7.909    2.829
12 KRAFT RB    2.229+-    3.455    -.031+-    6.302    1.564
16 CEMENT    13.874+-    11.324    23.364+-    20.317    1.550
TOTAL:    81.908+-    25.267    81.884+-    43.046
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
35.00000+-    7.000/    75.00000+-    7.000/    110.00000+-    9.899
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>C
ENTER COMMAND

```

Note that the user replied "SAME" to the question "DO YOU WANT RIDGE SOLUTIONS?" The user wishes to use the same analysis method as in the previous CMB command. Thus, the user has asked for ridge solutions, no ridge summary, a selection weight of 1.0, no effective variances, and an intercept included in the model. Using the SAME reply can eliminate repetitive replies if the user chooses to use a consistent analysis method.

The user issues a WRITE command to record the output on hardcopy. The hardcopy output from this session is given in Appendix C. The hardcopy output includes tables similar to the source coefficient table and the

calculated concentration table. Note that the latter will be included on the hardcopy even though it was not printed at the user's terminal.

```
>WRITE  
WRITTEN  
ENTER COMMAND
```

The user now would like to see the same analysis of the coarse fraction but with "background" removed. He gives the BACKOUT command and selects a background concentration receptor.

```
>BACKOUT  
ENTER BACKGROUND CMB SITE CODE: XXXXXXXXXXXX  
>BACKGROUND  
ENTER YEAR: YY  
>81  
ENTER DATE: MMDD  
>0229  
SITE: URBAN CORE      YEAR: 81  DATE: 0229  FC  
SITE: BACKGROUND     YEAR: 81  DATE: 0229  FC  
BACKOUT COMPLETE  
ENTER COMMAND
```

Now the user gives the CMB command to perform the analysis with background removed.

```
>CMB  
DO YOU WANT RIDGE SOLUTIONS?  
>SAME
```

```

CMB SITE: URBAN CORE      YEAR: 81    DATE: 0229    FRACTION: COARSE
SAMPLE DURATION: 12 WITH START HOUR: 7 BACKGROUND: YES EFF VAR: NO
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .4954    RIDGE K= .800      R-SQUARE: .6667
-----SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .010+-    .004      .021+-    .008
1 SOIL      21.685+-    13.296      56.462+-    63.335    6.733
2 RD DUST      8.110+-    4.089      9.703+-    9.882    2.465
3 SEA SALT      .192+-    .300      .428+-    .543    1.423
5 AUTO CAT      6.265+-    9.969      -48.147+-    51.722    7.508
6 AUTO      .256+-    .207      .350+-    .313    1.059
11 COAL      3.435+-    2.114      9.835+-    6.250    3.414
12 KRAFT RB      2.065+-    2.730      -.074+-    5.670    1.772
16 CEMENT      8.208+-    7.614      14.206+-    14.487    1.575
TOTAL:      50.225+-    21.945      42.783+-    37.577
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
7.00000+-    7.616/    38.00000+-    8.062/    45.00000+-    11.091
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
/C
ENTER COMMAND

```

Note that the user again uses the reply SAME to eliminate repetition in asking for the same analysis method as previously.

The BACKIN command removes the effect of the BACKOUT command. This may be desired if a reanalysis of the raw site data is desired or if the user would like to try another background site.

```

>BACKIN
BACKIN COMPLETE
ENTER COMMAND

```

The next command given by the user is AUTOFIT, so the BACKIN command was not actually necessary in this case. The AUTOFIT command will sequence through both size fractions of a selected receptor and all subsequent receptors on the Receptor Concentration Data File. It also writes the results to the hardcopy.

```

>AUTOFIT
ENTER DESIRED CMB SITE CODE: XXXXXXXXXXXX
>URBAN CORE
ENTER YEAR: YY
>81
ENTER DATE: MMDD
>0229
DATA SEARCH BEGUN FOR
    SITE: URBAN CORE      YEAR: 81  DATE: 0229

    SITE: URBAN CORE      YEAR: 81  DATE: 0229      FC
DO YOU WANT RIDGE SOLUTIONS?
>YES
CMB WILL SELECT THE BEST RIDGE SOLUTION
DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?
>NO
IN THE SELECTION OF THE BEST RIDGE SOLUTION,
WHAT WEIGHT DO YOU WANT? (DEFAULT=1.0)
>
WEIGHT IS      1.000000000
DO YOU WANT TO USE EFFECTIVE VARIANCES?
>NO
NO
DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?
>YES

CMB SITE: URBAN CORE      YEAR: 81  DATE: 0229      FRACTION: FINE
SAMPLE DURATION: 12 WITH START HOUR: 7  BACKGROUND: NO  EFF VAR: NO
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .9179  RIDGE K= .010      R-SQUARE: .9200
-----SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .004+-      .004      .005+-      .006
1 SOIL      -.509+-      3.092      -8.858+-      27.313      432.869
2 RD DUST      -.024+-      .923      .891+-      3.239      29.638
3 SEA SALT      -.446+-      .171      -.533+-      .265      14.234
5 AUTO CAT      7.377+-      20.436      -2.525+-      58.257      79.398
6 AUTO      4.635+-      .941      4.800+-      .975      2.881
9 DIST OIL      3.596+-      6.614      6.549+-      10.723      14.366
10 RES GAS      1.015+-      5.311      15.427+-      49.140      413.108
11 COAL      1.771+-      1.348      2.192+-      2.462      9.374
13 ELARCFRN      .076+-      .454      .048+-      1.249      71.640
14 FERRMFR      .061+-      .250      .083+-      .612      24.698
16 CEMENT      7.403+-      2.919      7.999+-      4.322      6.798
17 PET FCC      8.221+-      12.252      9.410+-      41.216      77.121
19 SEC S04      -.187+-      11.012      -3.353+-      49.346      173.618
TOTAL:      32.991+-      15.162      32.136+-      50.953
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
35.00000+-      7.000/      75.00000+-      7.000/      110.00000+-      9.899

```

The user has entered information selecting the first site. He has also chosen the analysis method. The method chosen will be used for the remaining sites and size fractions for the AUTOFIT sequence.

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND

The program pauses for a reply to the above prompt. However, a "C" does not return the user to command mode. Instead the program follows the above CMB analysis of the fine fraction of URBAN CORE with the CMB analysis of the coarse fraction. Note also that hardcopy is "WRITTEN."

AC
WRITTEN

CMB SITE: URBAN CORE		YEAR: 81	DATE: 0229	FRACTION: COARSE	
SAMPLE DURATION: 12 WITH START HOUR:		7	BACKGROUND: NO	EFF VAR: NO	
-----RIDGE REGRESSION-----			-----WEIGHTED LEAST SQUARES-----		
R-SQUARE: .6151 RIDGE K= .800			R-SQUARE: .7702		
---SOURCE-----UG/M3-----			---UG/M3-----VIF-----		
INTERCEPT	.011+-	.005	.023+-	.010	
1 SOIL	36.445+-	18.752	77.894+-	81.347	6.178
2 RD DUST	13.578+-	6.185	18.281+-	13.310	2.184
3 SEA SALT	.177+-	.491	.365+-	.771	1.223
5 AUTO CAT	10.339+-	13.655	-51.096+-	63.596	6.754
6 AUTO	.722+-	.275	1.180+-	.395	1.054
11 COAL	4.532+-	3.137	11.906+-	7.909	2.829
12 KRAFT RB	2.229+-	3.455	-.031+-	6.302	1.564
16 CEMENT	13.874+-	11.324	23.364+-	20.317	1.550
TOTAL:	81.908+-	25.267	81.884+-	43.046	
MEASURED CONCENTRATION FINE/COARSE/TOTAL:					
35.00000+-	7.000/	75.00000+-	7.000/	110.00000+-	9.899

Note that the sources for the fine and coarse fractions are different. The sources (and species) used are the selections currently in effect for each size fraction. These were determined in the initialization phase and by AS, AE, DS, and DE commands.

The user decides to display the calculated concentrations for the coarse fraction of the URBAN CORE site.

PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND

```

>
-----MEAS-----CALC-----RATIO-----
1 TOTAL      *    75.000+- 7.000  81.908+-25.267  1.09+- .35 TOT
2 AL         *    1.951+- .422   1.125+- .229   .58+- .17 AL
3 AS         *    .004+- .004    .011+- .000   2.76+- 2.76 AS
4 BA         *    .371+- .023    .011+- .000   .03+- .00 BA
5 BR         *    .108+- .007    .073+- .015   .67+- .14 BR
6 CA         *   13.014+- 1.442   5.186+- .842   .40+- .08 CA
7 CD         *    < .001        .011+- .000  22.10+-44.19 CD
8 CL         *    .288+- .068    .212+- .031   .74+- .20 CL
9 CO         *    .015+- .003    .011+- .000   .74+- .15 CO
10 CR        *    .022+- .005    .022+- .003   .99+- .26 CR
11 CU        *    .018+- .002    .018+- .001   1.01+- .13 CU
12 FE        *    1.871+- .118   1.204+- .205   .64+- .12 FE
13 HG        *    < .002        .011+- .000  11.05+-22.10 HG
14 K         *    .517+- .072    .347+- .070   .67+- .17 K
15 MN        *    .088+- .008    .035+- .004   .40+- .06 MN
16 NI        *    .003+- .001    .018+- .001   5.83+- 1.99 NI
17 P         *    .102+- .040    .011+- .000   .11+- .04 P
18 PB        *    .346+- .024    .171+- .038   .49+- .12 PB
19 SO4       *    1.725+- .939    6.525+- 1.306   3.78+- 2.19 SO4
20 SB        *    .004+- .002    .011+- .000   2.76+- 1.38 SB
21 SI        *    8.652+- 1.987   6.335+- 1.048   .73+- .21 SI
22 SN        *    .005+- .002    .011+- .000   2.21+- .88 SN
23 SR        *    .030+- .003    .016+- .001   .54+- .07 SR
24 TI        *    .205+- .037    .181+- .035   .88+- .23 TI
25 V         *    < .014        .015+- .001   2.10+- 4.21 V
26 ZN        *    .071+- .006    .054+- .008   .76+- .13 ZN
27 C         M    < .001        8.129+- 1.224   .00+- .00 C
28 NA        M    < .001        .422+- .068    .00+- .00 NA
29 NO3       M    < .001        .014+- .001    .00+- .00 NO3
30 RB        M    < .001        .012+- .000    .00+- .00 RB
31 SE        M    < .001        .011+- .000    .00+- .00 SE
>

```

WRITTEN
WRITTEN

Note that the program paused at the end of the table display. The user gave a RETURN to continue processing. The program replied with two "WRITTEN" messages, indicating that the coarse fraction results have been written to hardcopy and that a site summary report has been written. The User Followup Data File was also written upon at this point.

The program now proceeds to the next site. First it brings in the concentration data, then displays the analysis.

```

DATA SEARCH BEGUN FOR
  SITE: BACKGROUND      YEAR: 81  DATE: 0229

  SITE: URBAN CORE      YEAR: 81  DATE: 0229      FC
  SITE: BACKGROUND      YEAR: 81  DATE: 0229      FC

CMB SITE: BACKGROUND    YEAR: 81  DATE: 0229      FRACTION: FINE
SAMPLE DURATION: 12 WITH START HOUR: 7 BACKGROUND: NO EFF VAR: NO
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .8287  RIDGE K= .120      R-SQUARE: .9241
---SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .006+- .006      .005+- .006
1 SOIL      -.334+- .346      -14.654+- 34.854 7594.633
2 RD DUST      .214+- .656      1.231+- 3.814 91.330
3 SEA SALT      -.187+- .093      -.667+- .264 19.554
5 AUTO CAT      12.538+- 7.325      -26.438+- 39.874 52.511
6 AUTO      1.889+- .609      2.261+- .522 1.823
9 DIST OIL      1.572+- 3.786      20.923+- 12.055 25.512
10 RES GAS      -.735+- .733      17.660+- 61.095 6725.402
11 COAL      1.088+- .951      3.035+- 2.132 13.675
13 ELARCFRN      -.053+- .114      -.117+- .974 93.757
14 FERRMFR      .147+- .137      .186+- .498 22.554
16 CEMENT      2.884+- 1.166      9.390+- 3.855 30.223
17 PET FCC      4.596+- 4.504      6.337+- 24.170 55.903
19 SEC SO4      4.025+- 4.481      7.995+- 30.701 78.138
TOTAL:      27.650+- 7.882      27.147+- 20.851
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
28.00000+- 3.000/ 37.00000+- 4.000/ 65.00000+- 5.000

```

The user decides to stop the AUTOFIT sequence and return to command mode.

```
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>STOP
ENTER COMMAND
```

The user is now in command mode and may enter any valid command. However, he decides that he would like to continue the AUTOFIT sequence after all. He enters the RESUME command and the programs takes up the AUTOFIT sequence where it left off.

```
>RESUME
WRITTEN
```

```
CMB SITE: BACKGROUND      YEAR: 81    DATE: 0229    FRACTION: COARSE
SAMPLE DURATION: 12 WITH START HOUR: 7  BACKGROUND: NO  EFF VAR: NO
-----RIDGE REGRESSION-----    -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .8785    RIDGE K= .480    R-SQUARE: .9570
-----SOURCE-----UG/M3-----    -----UG/M3-----VIF-----
INTERCEPT    .003+-    .002    .003+-    .003
1 SOIL    20.253+-    5.861    27.211+-    16.919    7.651
2 RD DUST    6.130+-    1.363    7.989+-    2.435    3.687
3 SEA SALT    -.024+-    .031    -.053+-    .114    10.065
5 AUTO CAT    1.749+-    4.822    -9.926+-    14.544    8.157
6 AUTO    .540+-    .106    .820+-    .099    1.130
11 COAL    1.397+-    .840    2.655+-    1.708    4.580
12 KRAFT RB    .053+-    .538    -.156+-    2.073    10.701
16 CEMENT    6.954+-    2.694    9.610+-    3.288    1.852
TOTAL:    37.055+-    13.502    38.153+-    21.236
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
28.00000+-    3.000/    37.00000+-    4.000/    65.00000+-    5.000
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>C
WRITTEN
WRITTEN
AUTOFIT SEQUENCING FINISHED
ENTER COMMAND
```

The program has noted that the AUTOFIT sequence is finished.

The user would now like to average the previous analyses across sites (or dates if there were multiple dates). This is done with the PCOMP command. Only site analyses which were followed by the double "WRITTEN" message are included. Ordinarily, the results to be averaged are of a comparable nature, e.g., averages could be computed for a set of sites in the urban core for one or more dates. However, averaging the urban core and background sites illustrates the mechanics.

PCOMP
 OUTPUT WILL GO TO HARDCOPY.
 DO YOU WANT IT DISPLAYED AT YOUR TERMINAL INSTEAD?
 >YES

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	SOIL	-.51	36.45	35.94
BACKGROUND	81/02/29	SOIL	-.33	20.25	19.92
		AVERAGE	-.42	28.35	27.93
		(STD. DEV.)	+-.12	+-.11.45	+-.11.33

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	RD DUST	-.02	13.58	13.55
BACKGROUND	81/02/29	RD DUST	.21	6.13	6.34
		AVERAGE	.10	9.85	9.95
		(STD. DEV.)	+-.17	+-.5.27	+-.5.10

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL ² (UG/M3)
URBAN CORE	81/02/29	SEA SALT	-.45	.18	-.27
BACKGROUND	81/02/29	SEA SALT	-.19	-.02	-.21
			-----	-----	-----
		AVERAGE	-.32	.08	-.24
		(STD. DEV.) +- .18		+- .14	+- .04

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	AUTO CAT	7.38	10.34	17.72
BACKGROUND	81/02/29	AUTO CAT	12.54	1.75	14.29
			-----	-----	-----
		AVERAGE	9.96	6.04	16.00
		(STD. DEV.) +- 3.65		+- 6.07	+- 2.43

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	AUTO	4.63	.72	5.36
BACKGROUND	81/02/29	AUTO	1.89	.54	2.43
			-----	-----	-----
		AVERAGE	3.26	.63	3.89
		(STD. DEV.) +- 1.94		+- .13	+- 2.07

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	DIST OIL	3.60	.00	3.60
BACKGROUND	81/02/29	DIST OIL	1.57	.00	1.57
			-----	-----	-----
		AVERAGE	2.58	.00	2.58
		(STD. DEV.) +- 1.43		+- .00	+- 1.43

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	RES GAS	1.02	.00	1.02
BACKGROUND	81/02/29	RES GAS	-.73	.00	-.73
	AVERAGE		.14	.00	.14
	(STD. DEV.)	+-	1.24	+- .00	+- 1.24

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	COAL	1.77	4.53	6.30
BACKGROUND	81/02/29	COAL	1.09	1.40	2.49
	AVERAGE		1.43	2.96	4.39
	(STD. DEV.)	+-	.48	+- 2.22	+- 2.70

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	KRAFT RB	.00	2.23	2.23
BACKGROUND	81/02/29	KRAFT RB	.00	.05	.05
	AVERAGE		.00	1.14	1.14
	(STD. DEV.)	+-	.00	+- 1.54	+- 1.54

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	ELARCFRN	.08	.00	.08
BACKGROUND	81/02/29	ELARCFRN	-.05	.00	-.05
	AVERAGE		.01	.00	.01
	(STD. DEV.)	+-	.09	+- .00	+- .09

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	FERRMNFR	.06	.00	.06
BACKGROUND	81/02/29	FERRMNFR	.15	.00	.15
AVERAGE			.10	.00	.10
(STD. DEV.)			+-.06	+-.00	+-.06

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	CEMENT	7.40	13.87	21.28
BACKGROUND	81/02/29	CEMENT	2.88	6.95	9.84
AVERAGE			5.14	10.41	15.56
(STD. DEV.)			+-.3.20	+-.4.89	+-.8.09

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	PET FCC	8.22	.00	8.22
BACKGROUND	81/02/29	PET FCC	4.60	.00	4.60
AVERAGE			6.41	.00	6.41
(STD. DEV.)			+-.2.56	+-.00	+-.2.56

CMB SITE	DATE	SOURCE	FINE (UG/M3)	COARSE (UG/M3)	TOTAL (UG/M3)
URBAN CORE	81/02/29	SEC S04	-.19	.00	-.19
BACKGROUND	81/02/29	SEC S04	4.02	.00	4.02
AVERAGE			1.92	.00	1.92
(STD. DEV.)			+-.2.98	+-.00	+-.2.98

ENTER COMMAND

The user would like to know what the current status is. That is, what are the current site, size fraction, sources, and species. He enters the PINFO command.

```
>PINFO
***CURRENT STATUS***
CMB SITE: BACKGROUND      YEAR: 81   DATE: 0229
COARSE SIZE FRACTION
DURATION: 12  START HOUR: 7
HAS BACKGROUND BEEN SUBTRACTED: NO
FITTING SPECIES
  1  TOTAL
  2  AL
  4  BA
  5  BR
  6  CA
  8  CL
  9  CO
 10  CR
 11  CU
 12  FE
 14  K
 15  MN
 17  P
 18  PB
 21  SI
 23  SR
 24  TI
 26  ZN
FITTING SOURCES
  1  SOIL
  2  RD DUST
  3  SEA SALT
  5  AUTO CAT
  6  AUTO
 11  COAL
 12  KRAFT RB
 16  CEMENT
ENTER COMMAND
```

This shows that the last site and size fraction analyzed in the AUTOFIT sequence is current.

The user decides to do an alternate analysis. He chooses ridge regression as before, but he asks for the summary of all solutions. He also sets the weight to 10.0, favoring the selection of a solution without significant negative coefficients. Also, he chooses the effective variance option.

```
>CMB
DO YOU WANT RIDGE SOLUTIONS?
>Y
CMB WILL SELECT THE BEST RIDGE SOLUTION
DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?
>Y
IN THE SELECTION OF THE BEST RIDGE SOLUTION,
WHAT WEIGHT DO YOU WANT? (DEFAULT=1.0)
>10.
WEIGHT IS          10.000000000
DO YOU WANT TO USE EFFECTIVE VARIANCES?
>Y
DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?
>Y
```

Note that the user does not spell out "YES" but instead merely gives a "Y." He could also use "N" for "NO." The first letter can be used for most replies to the CMB program queries. It cannot be used for COMMANDS.

The CMB program now displays the summary of solutions.

RIDGE K	R-SQUARE	AEROSOL	SE (AEROSOL)	# NEG	WORST	ITERATIONS
.000	.8837	37.315	16.01	3	-6.547	3
.005	.8836	37.293	15.91	3	-5.666	2
.010	.8837	37.276	15.83	3	-4.919	2
.015	.8838	37.263	15.75	3	-4.267	2
.020	.8838	37.253	15.67	3	-3.692	2
.025	.8839	37.244	15.60	3	-3.181	2
.030	.8839	37.236	15.52	3	-2.723	2
.035	.8839	37.229	15.45	3	-2.310	2
.040	.8839	37.222	15.38	3	-1.936	2
.045	.8838	37.215	15.31	3	-1.596	2
.050	.8838	37.208	15.24	3	-1.284	2
.060	.8837	37.192	15.11	3	-.735	2
.070	.8835	37.175	14.99	3	-.274	2
.080	.8832	37.154	14.87	2	-.271	2
.090	.8829	37.131	14.75	2	-.267	2
.100	.8826	37.104	14.64	2	-.262	2
.120	.8817	37.042	14.42	2	-.252	2
.140	.8806	36.969	14.22	2	-.240	2
.160	.8793	36.885	14.03	2	-.228	2
.180	.8778	36.792	13.85	2	-.216	2
.200	.8762	36.691	13.68	2	-.204	2
.240	.8725	36.469	13.37	2	-.181	2
.280	.8682	36.226	13.08	2	-.159	2
.320	.8635	35.966	12.82	2	-.139	2
.360	.8584	35.693	12.58	2	-.120	2
.400	.8530	35.412	12.35	2	-.103	2
.480	.8414	34.832	11.93	2	-.072	2
.560	.8291	34.241	11.56	2	-.046	2
.640	.8164	33.649	11.22	2	-.023	2
.720	.8033	33.062	10.90	2	-.013	2
.800	.7900	32.483	10.61	1	-.012	2

RIDGE K= .180 IS THE SELECTED BEST SOLUTION

The R^2 value is given for each value of the ridge K. The calculated total aerosol mass and its standard error are also given. The program tries to find a solution with this calculated value close to the measured value, which is $35 \mu\text{g}/\text{m}^3$ in this case. The number of negative coefficients is also given along with the value of the negative coefficient of greatest magnitude. Finally, the number of iterations in the effective variance procedure is given.

In conventional ridge regression, the R^2 value is highest for the case when $k = 0$. Due to certain required data transformations discussed in Appendix D, however, R^2 may oscillate in some cases as k increases if effective variances are used. The R^2 value is a measure of the agreement between observed and predicted concentrations after the variance stabilizing transformation.

Next the CMB program displays the chosen best solution.

```

CMB SITE: BACKGROUND      YEAR: 81    DATE: 0229    FRACTION: COARSE
SAMPLE DURATION: 12 WITH START HOUR: 7 BACKGROUND: NO  EFF VAR: YES
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .8778    RIDGE K= .180      R-SQUARE: .8837
-----SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .003+-    .002      .004+-    .003
1 SOIL            15.349+-    6.147      22.079+-    19.624    9.394
2 RD DUST         7.963+-    2.190      8.616+-    3.282    1.881
3 SEA SALT        -.031+-    .047      -.054+-    .120    4.668
5 AUTO CAT        2.453+-    4.943      -6.547+-    16.549    8.510
6 AUTO            .687+-    .206      .847+-    .286    1.261
11 COAL           1.255+-    .925      2.268+-    2.178    2.815
12 KRAFT RB       -.216+-    .794      -.203+-    1.980    4.853
16 CEMENT         9.329+-    3.380      10.305+-    5.092    2.009
TOTAL:           36.792+-    13.852      37.315+-    16.005
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
28.00000+-    3.000/    37.00000+-    4.000/    65.00000+-    5.000
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>C
ENTER COMMAND

```

The user would like to look at all of the solutions. He therefore enters the PSOLN command.

```

PSOLN
THERE ARE 31 SOLUTIONS WITH AN INTERCEPT
AND 8 SOURCE COEFFICIENTS AND STANDARD ERRORS
EACH FOR 527 NUMBERS TOTAL.
THEY CAN PRINT TO YOUR TERMINAL OR TO HARD COPY.
ARE YOU SURE YOU WANT TO LOOK AT THESE NUMBERS?
>Y
DO YOU WANT THE SOLUTIONS PRINTED ON THE HARD COPY
(INSTEAD OF AT YOUR TERMINAL)?
>Y
SOLUTIONS WRITTEN TO HARD COPY
ENTER COMMAND

```

Recognizing the volume of data in the display, the user has elected to send the results to the hardcopy. The results are included in Appendix C. Note that the user is continuing to use shorthand replies.

The user would like to check some of the input data. He enters the PMATRIX command.

```

>PMATRIX
MATRICES CAN GO TO HARD COPY
DO YOU WANT THEM DISPLAYED AT YOUR TERMINAL INSTEAD?
>Y
WHAT DO YOU WANT TO SEE?
SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS, OR CODES?
>RECEPTORS

```

The user spelled out "RECEPTORS," but the abbreviation "R" could have been used. The display is as follows:

CURRENT MEASURED UG/M3 CONCENTRATIONS FOR
 SITE:BACKGROUND YEAR: 81 DATE: 0229

SPECIES	FINE		COARSE		TOTAL	
1 TOTAL	28.000+-	3.000	37.000+-	4.000	65.000+-	5.000
2 AL	.070+-	.055	.739+-	.171	.809+-	.180
3 AS	.014+-	.006	.001+-	.004	.015+-	.007
4 BA	.146+-	.018	.086+-	.016	.232+-	.024
5 BR	.164+-	.010	.064+-	.005	.228+-	.011
6 CA	.128+-	.008	3.805+-	.444	3.933+-	.444
7 CD	.001+-	.002	.001+-	.002	.002+-	.003
8 CL	.010+-	.007	.014+-	.010	.024+-	.012
9 CO	.008+-	.003	.001+-	.003	.009+-	.004
10 CR	.010+-	.005	.003+-	.005	.012+-	.007
11 CU	.027+-	.003	.004+-	.002	.031+-	.004
12 FE	.120+-	.008	.692+-	.044	.812+-	.045
13 HG	.001+-	.003	.009+-	.003	.010+-	.004
14 K	.186+-	.010	.215+-	.032	.401+-	.034
15 MN	.022+-	.004	.018+-	.004	.040+-	.006
16 NI	.003+-	.002	.001+-	.002	.004+-	.003
17 P	.103+-	.018	.020+-	.022	.123+-	.028
18 PB	.894+-	.047	.213+-	.017	1.107+-	.050
19 SO4	14.780+-	.765	.852+-	.783	15.632+-	1.095
20 SB	.008+-	.003	.001+-	.003	.009+-	.004
21 SI	.189+-	.027	4.000+-	.914	4.189+-	.914
22 SN	.024+-	.003	.003+-	.003	.027+-	.004
23 SR	.003+-	.002	.006+-	.002	.009+-	.003
24 TI	.008+-	.016	.097+-	.017	.105+-	.023
25 V	.003+-	.009	.003+-	.007	.006+-	.011
26 ZN	.038+-	.003	.016+-	.003	.054+-	.004
27 C	.000+-	.001	.000+-	.001	.000+-	.001
28 NA	.000+-	.001	.000+-	.001	.000+-	.001
29 NO3	.000+-	.001	.000+-	.001	.000+-	.001
30 RB	.000+-	.001	.000+-	.001	.000+-	.001
31 SE	.000+-	.001	.000+-	.001	.000+-	.001

The CMB program again asks the user what input data should be displayed. This time the user selects the source signature matrix. However, he only wishes to look at one of the sources, not the entire matrix:

WHAT DO YOU WANT TO SEE?
 SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS, OR CODES?
 OR ARE YOU DONE?

>SOURCES

WHAT SIZE FRACTION? (FINE OR COARSE)

>C

DO YOU WANT TO LOOK AT THE WHOLE MATRIX?

IT IS 19 SOURCES BY 31 SPECIES

>N

WHICH SOURCE DO YOU WANT?

GIVE SOURCE #

>2

SOURCE: RD DUST

1 TOTAL	1.0000	+-	.0000
2 AL	.0659	+-	.0165
3 AS	.0000	+-	.0000
4 BA	.0000	+-	.0000
5 BR	.0001	+-	.0000
6 CA	.0300	+-	.0075
7 CD	.0000	+-	.0000
8 CL	.0000	+-	.0000
9 CO	.0000	+-	.0000
10 CR	.0000	+-	.0000
11 CU	.0000	+-	.0000
12 FE	.0573	+-	.0143
13 HG	.0000	+-	.0000
14 K	.0000	+-	.0000
15 MN	.0010	+-	.0003
16 NI	.0000	+-	.0000
17 P	.0000	+-	.0000
18 PB	.0000	+-	.0000
19 SO4	.0000	+-	.0000
20 SB	.0000	+-	.0000
21 SI	.2840	+-	.0710
22 SN	.0000	+-	.0000
23 SR	.0000	+-	.0000
24 TI	.0101	+-	.0025
25 V	.0003	+-	.0001
26 ZN	.0000	+-	.0000
27 C	.0489	+-	.0122
28 NA	.0175	+-	.0044
29 NO3	.0002	+-	.0001
30 RB	.0000	+-	.0000
31 SE	.0000	+-	.0000

```

WHICH SOURCE DO YOU WANT?
GIVE SOURCE #
>
WHAT DO YOU WANT TO SEE?
SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS, OR CODES?
OR ARE YOU DONE?
>DONE
ENTER COMMAND

```

Since the user only wanted to look at the Road Dust source signature, he gave a RETURN when asked for the next source. Furthermore, since he was finished examining input data, he returned to command mode.

Now the user employs the INITIAL command to restore the original selection of sources and species for the coarse size fraction. This returns the coarse source and species lists to their condition at the end of the initialization phase.

```

>INITIAL
SIZE IS COARSE
ENTER COMMAND

```

Now the user does a CMB analysis on the coarse fraction of the "Background" site without using the ridge option. Note that the "ridge" results and the least squares solution are identical.

```

>CMB
DO YOU WANT RIDGE SOLUTIONS?
>N
DO YOU WANT TO USE EFFECTIVE VARIANCES?
>N
DO YOU WANT TO INCLUDE THE INTERCEPT IN THE MODEL?
>N

```

```

CMB SITE: BACKGROUND      YEAR: 81    DATE: 0229    FRACTION: COARSE
SAMPLE DURATION: 12 WITH START HOUR: 7 BACKGROUND: NO EFF VAR: NO
-----RIDGE REGRESSION-----      -----WEIGHTED LEAST SQUARES-----
R-SQUARE: .9553    RIDGE K= .000      R-SQUARE: .9553
---SOURCE-----UG/M3-----      -----UG/M3-----VIF-----
INTERCEPT      .000+-      .000      .000+-      .000
1 SOIL            80.412+-  80.592      80.412+-  80.592  110.800
2 RD DUST         5.407+-   8.682      5.407+-   8.682   27.837
3 SEA SALT        .863+-   1.132      .863+-   1.132   691.696
5 AUTO CAT       54.731+-  69.153      54.731+-  69.153  420.117
6 AUTO           .850+-   .117      .850+-   .117    1.109
7 JET AIR        -17.418+- 53.437      -17.418+- 53.437   31.827
9 DIST OIL       -13.134+- 18.948      -13.134+- 18.948  187.619
10 RES GAS       -50.557+- 67.151      -50.557+- 67.151  350.204
11 COAL          -15.310+- 21.876      -15.310+- 21.876   81.796
12 KRAFT RB      -10.988+- 13.717      -10.988+- 13.717  366.998
13 ELARCFRN      2.736+-   3.373      2.736+-   3.373 1338.700
14 FERRMFR       -9.637+- 11.824      -9.637+- 11.824 1205.257
16 CEMENT        11.503+-   9.054      11.503+-   9.054   9.787
17 PET FCC       -2.459+- 14.132      -2.459+- 14.132   4.676
TOTAL:           37.000+- 21.769      37.000+- 21.769
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
28.00000+- 3.000/ 37.00000+- 4.000/ 65.00000+- 5.000
PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT COMMAND
>C
ENTER COMMAND

```

Since the user did not ask for ridge solutions, the "ridge" solution on the left is identical to the least squares solution on the right. The user also chose not to include the intercept in the model. Therefore, the intercept is set exactly to zero. It is apparent from the negative values with large magnitudes and the large standard errors that conventional weighted least squares is inadequate to handle this complex set of sources. It is clear from the variance inflation factors that this case is strongly affected by multicollinearity. As is discussed in Section 2, reducing the number of sources and using the ridge feature are two possible approaches for obtaining a reasonable solution.

Now the user has completed his session and enters the EXIT command to end it.

```
>EXIT
```

The session is now over.

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APPENDIX A
SOURCE PROGRAM LISTINGS

This appendix gives the FORTRAN source program listings of the CMB main program and subprograms. These programs and their functions are as follows:

MAIN	Program control and output
CMBR	Perform CMB analysis
FETCH	Search receptor concentration data file for selected site/date
INVL	Matrix inversion
COARS	Compute coarse fraction from Total and Fine fractions
PERC	Compute component percentages

TABLE A.1 CMB MAIN PROGRAM

```

1  C
2  C  PROGRAM CMB MAIN
3  C
4  C
5  C
6  C  THIS PROGRAM WAS ADAPTED FROM THE CMBDEQ
7  C PROGRAM DEVELOPED FOR THE STATE OF OREGON DEQ
8  C BY THE OREGON GRADUATE CENTER FOR STUDY AND RESEARCH.
9  C THE PROGRAM IS BASED ON THE WORK OF DR. J. WATSON'S CEB2 CODE
10 C AS MODIFIED BY D. TORKELOSON AS THE CMBDEQ CODE. THIS
11 C ADAPTATION WAS DEVELOPED BY J. CORE AND W. HAMILTON
12 C OF THE US EPA, OAQPS, RTP. N. CAROLINA, 1981.
13 C THE PROGRAM WAS ORIGINALLY WRITTEN FOR THE PRIME 350
14 C AND ADAPTED TO THE EPA'S SPERRY UNIVAC 1100 SYSTEM.
15 C  PROGRAM VARIABLES
16 C AND NECESSARY INPUT/OUTPUT FILES ARE DESCRIBED BELOW.
17 C
18 C  IN 1982, THE CMB MAIN PROGRAM AND THE SUBPROGRAM
19 C FETCH WERE MODIFIED AND ENHANCED. THE NEW
20 C SUBPROGRAM CMBR REPLACED CEB2,
21 C THEREBY ADDING A RIDGE REGRESSION OPTION.
22 C THIS WORK WAS DONE UNDER CONTRACT TO US EPA
23 C BY DR. H.J. WILLIAMSON AND DR. D.A. DUBOSE
24 C RADIANT CORP. AUSTIN, TEXAS
25 C EPA PROJECT OFFICER: W.P. FREAS
26 C
27 C
28 C
29 C *****
30 C
31 C      REQUIRED INPUT FILES-
32 C
33 C      UNIT2, SONM - FILE OF SOURCE CODES AND
34 C                   SOURCE MNEMONICS. THIS FILE DEFINES THE
35 C                   SOURCES IN THE WORKING SOURCE MATRIX.
36 C
37 C      UNIT3, PONM - FILE OF POLLUTANT CODES AND
38 C                   POLLUTANT MNEMONICS. THIS FILE DEFINES THE
39 C                   POLLUTANTS IN THE WORKING SOURCE MATRIX.
40 C
41 C      UNIT7, SORF - FILE OF FRACTIONAL POLLUTANT COMPOSITIONS
42 C                   FOR FINE FRACTION SOURCES SIGNATURES
43 C
44 C      UNIT8, SORC - FILE OF FRACTIONAL POLLUTANT COMPOSITIONS
45 C                   FOR COARSE FRACTION SOURCES SIGNATURES
46 C
47 C      UNIT13, DATA - FILE OF FINE AND TOTAL FRACTION AMBIENT DATA
48 C                   RECEPTOR CONCENTRATION DATA

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

49 C
50 C
51 C     OUTPUT DISK FILES-
52 C
53 C
54 C     UNIT11, CMBOUT - FILE OF FINE, COARSE AND TOTAL
55 C                   CMB RESULTS INCLUDING CHEMICAL AND FIT DATA.
56 C                   GENERAL PRINT FILE
57 C                   OPTIONAL OUTPUT FROM COMMANDS PMATRIX,PCOMP,PSOLN
58 C
59 C     UNIT 9, SUMMRY - FILE OF SUMMARIZED FINE , COARSE AND TOTAL
60 C                   SOURCE COTRIBUTIONS
61 C                   SUMMARY PRINT FILE
62 C
63 C     UNIT12, MAGSTO - FILE OF INPUT CARD DATA PLUS MASS AND
64 C                   POLLUTANT CONTRIBUTIONS FOR EACH SOURCE.
65 C                   USER FOLLOW UP FILE
66 C
67 C     UNIT10,TEMP - FILE OF TEMPORARY INPUT DATA STORAGE
68 C
69 C     INTERACTIVE TERMINAL FILES
70 C
71 C     UNIT5 - TERMINAL READ
72 C
73 C     UNIT6 - TERMINAL WRITE
74 C *****
75 C
76 C
77 C *****VARIABLE NAMES*****
78 C
79 C     WORD HOLDER DATA ARRAYS
80 C     ELMNT(IEL)-ELEMENT MNEMONICS
81 C     SOUNAM(JSOURC)-SOURCE MNEMONICS
82 C     COMAND(ICMND)-COMMANDS
83 C     COMND1-COMMAND READ FROM SCREEN
84 C     SIZNAM-SAMPLE FRACTION DESCRIPTION
85 C     YBACK- CURRENT BACKGROUND SUBTRACTION INDICATOR
86 C     TEMPN- TEMPORARY NAME MATCHING HOLDER
87 C     STNM-CURRENT SITE NAME
88 C     BSTNM-CURRENT BACKGROUND SITE NAME
89 C
90 C
91 C     SOURCE COMPOSITION ARRAYS
92 C     A(IEL,JSOURC,ISIZ)-SOURCE COMPOSITIONS
93 C     UA(IEL,JSOURC,ISIZ)-UNCERTAINTIES OF A
94 C     SCODE(JSOURC)- SOURCE CODES
95 C     PCODE(IEL)- POLLUTANT CODES
96 C

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```
97 C
98 C COUNTERS AND LIMITS
99 C I-GENERAL COUNTER
100 C IEL-ELEMENT COUNTER
101 C KEL-FITTING ELEMENT COUNTER
102 C LEL-ELEMENT DELETE COUNTER
103 C NEL-TOTAL NUMBER OF SOURCE QUANTIFIED ELEMENTS
104 C MEL-NUMBER OF FITTING ELEMENTS
105 C JSOURC-SOURCE COUNTER
106 C KSOURC-FITTING SOURCE COUNTER
107 C LSOURC-SOURCE DELETE COUNTER
108 C NSOURC-TOTAL NUMBER OF SOURCES
109 C MSOURC-NUMBER OF FITTING SOURCES
110 C IFLAG-METHOD FLAG COUNTER(INVERSION ERROR)
111 C ICMND-COMMAND COUNTER
112 C NCMND-TOTAL NUMBER OF COMMANDS
113 C MELMAX-MAXIMUM NUMBER OF FITTING ELEMENTS
114 C MSOMAX-MAXIMUM NUMBER OF FITTING SOURCES
115 C MSOMIX-MSOMAX LESS ONE TO ALLOW FOR INTERCEPT
116 C
117 C
118 C
119 C
120 C SAMPLE IDENTIFICATION VARIABLES
121 C CMBID- UNIQUE DATA SET NUMBER OR NAME
122 C UDUR-SAMPLING DURATION IN HOURS
123 C USTART-SAMPLING START HOUR
124 C
125 C
126 C OPERATIONS VARIABLES
127 C UCNC(IEL,ISIZ)-URBAN OPERATIONS MEASURED CONCENTRATIONS
128 C UUCNC(IEL,ISIZ)-UNCERTAINTY OF UCNC
129 C CLCN(IEL,ISIZ)-CALCULATED CONCENTRATION
130 C UCLCN(IEL,ISIZ)-UNCERTAINTY OF CLCN
131 C UFMSS-URBAN FINE MASS LOADING
132 C UUFMSS-UNCERTAINTY OF UFMSS
133 C UCMSS- COARSE MASS
134 C UUCMSS - UNCERTAINTY
135 C UTMSS- TOTAL MASS
136 C UUTMSS- UNCERTAINTY
137 C MFLAG(IEL,3)-MISSING DATA FLAG FOR EACH ELEMENT AND SIZE
138 C
139 C
140 C BACKGROUND SUBTRACTION VARIABLES
141 C -SAME AS URBAN PREFACED WITH A 'B'
142 C
143 C
144 C
```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

145 C TEMPORARY OUTPUT VARIABLES
146 C PCNT-PERCENT
147 C UPCNT-UNCERTAINTY PERCENT
148 C FPCNT-FINE PERCENT
149 C UFPCNT-UNCERTAINTY
150 C CPCNT-COARSE PERCENT
151 C UCPCNT-UNCERT
152 C TPCNT-TOTAL PERCENT
153 C UTPCNT-UNCERTAINTY
154 C X-GENERAL
155 C UX-GENERAL
156 C TX-GENERAL TOTALS
157 C UTX-UNCERTAINTY
158 C RATIO-RATIO OF CALCULATED TO MEASURED
159 C URATIO-UNCERTAINTY OF RATIO
160 C
161 C
162 C
163 C FIT INITIALIZATION ARRAYS
164 C INTEL(IEL)-INITIAL FITTING ELEMENTS
165 C INITSO(JSOURC)-INITIAL FITTING SOURCES
166 C IMEL-NUMBER OF INITIAL FITTING ELEMENTS
167 C IMSO-NUMBER OF INITIAL FITTING SOURCES
168 C
169 C MISC.
170 C ELFT(IEL,ISIZ)-ELEMENT FITTING FLAG
171 C ELHOLD(KEL,ISIZ)-ELEMENT FITTING PLACE HOLDER
172 C SOUFT(JSOURC,ISIZ)-SOURCE FITTING FLAG
173 C SOHOLD(KSOURC,ISIZ)-SOURCE FITTING PLACE HOLDER
174 C IRTN-GO TO STATEMENT VARIABLE
175 C JRTN-GO TO STATEMENT VARIABLE
176 C UNITX-FORTRAN FILE UNIT NUMBER
177 C X-GENERAL REAL NUMBER
178 C ICNTRL-AUTOFIT/SELECT CONTROL CODE FOR FETCH
179 C SEL(ISIZ)-ELEMENTAL SOURCE CONTRIBUTIONS
180 C USEL(ISIZ)-UNCERTAINTY
181 C ISCTR-PRINTED SOURCE COUNTER
182 C ISHOLD(ISCTR)-ARRAY POSITIONS OF PRINTED SOURCES
183 C IBACK-CURRENT BACKGROUND SUBTRACTION INDICATOR
184 C DUM(20)-SCRATCH VECTOR
185 C SAVE-AUTOFIT TITLE LINE HOLDER
186 C
187 C
188 C BOOKKEEPING
189 C
190 C ANS-ANSWER TO PROGRAM QUERIES
191 C CHK-ANSWER TO PROGRAM QUERIES
192 C IBACK-BACKGROUND SUBTRACTION STATUS FLAG

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```
193 C IWIDE-TERMINAL LINE WIDTH FLAG
194 C LASTID-HOLDER FOR CMBID IN PCOMP
195 C LOOP -CYCLING STATUS FLAG IN PMATRIX
196 C MANY-LINE WIDTH CONTROL INDEX
197 C MORE-LINE WIDTH CONTROL INDEX
198 C NOSKIP-CMB PARAMETER CONTROL FLAG CONTROLLED BY AUTOFIT
199 C OLDID-HOLDER FOR CMBID TO PREVENT TOTALING FINE AND COARSE
200 C OF DIFFERENT SITES IN WRITE
201 C PNAME-ARRAY FOR CMBID'S IN PCOMP
202 C SITE-SITE CODE :
203 C YEAR-YEAR : COMPONENTS OF CMBID
204 C DATE-MONTH AND DAY :
205 C SPACE-DUMMY CHARACTER FOR READ
206 C TEMPID-TEMPORARY HOLDER FOR CMBID CHECK
207 C
208 C
209 C
210 C CMBR SUBPROGRAM ARGUMENTS AND RELATED VARIABLES
211 C
212 C AP-CMBR WORK SPACE
213 C C-RECEPTOR CONCENTRATION VECTOR
214 C CWT-WEIGHT FOR SELECTING RIDGE SOLUTIONS
215 C CWT10-TEMPORARY HOLDER FOR CWT VALUE
216 C EFVAR-EFFECTIVE VARIANCE FLAG
217 C SELK-LEAST SQUARES SOLUTION
218 C F-SOURCE SIGNATURE MATRIX
219 C IA-CMBR WORK SPACE
220 C INTCEP-INTERCEPT OPTION FLAG
221 C IS-CMBR WORK SPACE
222 C ITM-CMBR WORK SPACE
223 C KINDEX-INDEX OF SELECTED BEST RIDGE SOLUTION
224 C R2LS-R-SQUARE FOR LEAST SQUARES SOLUTION
225 C RIDGE -RIDGE OPTION FLAG
226 C S-CMBR WORK SPACE
227 C SAINT-SELECTED RIDGE SOLUTION INTERCEPT
228 C SAINTO-LEAST SQUARES SOLUTION VECTOR
229 C SAS-RIDGE SOLUTION MATRIX
230 C SAA-RIDGE SOLUTION STANDARD ERROR MATRIX
231 C SET-STANDARD ERROR OF CALCULATED TOTAL AEROSOL
232 C SETLS-STANDARD ERROR OF CALCULATED TOTAL AEROSOL(LEAST SQUARES)
233 C SF-STANDARD ERROR OF SOURCE SIGNATURE MATRIX
234 C SOLD-CMBR WORK SPACE
235 C SR2-R-SQUARE FOR SELECTED RIDGE SOLUTION
236 C SSET-STANDARD ERROR OF CALCULATED TOTAL AEROSOL
237 C SX-CMBR WORK SPACE
238 C USAINT-UNCERTAINTY OF SAINT (RIDGE SOLN INTERCEPT)
239 C USAINO-UNCERTAINTY OF SAINTO (LEAST SQUARES INTERCEPT)
240 C VELK-STANDARD ERROR OF LEAST SQUARES SOLUTION
```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

241 C TM-WORK VECTOR FOR CMBR
242 C TOTALA-TOTAL AEROSOL MASS
243 C V-STANDARD ERRORS OF RECEPTOR CONCENTRATION VECTOR
244 C VIF-VARIANCE INFLATION FACTOR
245 C VIFELK-VIF ORGANIZED BY SOURCE INDECIES
246 C VK-VECTOR OF K-VALUES FOR RIDGE REGRESSION
247 C XMEAN-USED BY CMBR FOR SOURCE MEANS
248 C XP-USED BY CMBR FOR X MATRIX
249 C XPX-USED BY CMBR FOR X'X MATRIX
250 C XPXK-USED BY CMBR FOR X'X MATRIX(INVERSE)
251 C XPY-USED BY CMBR FOR X'Y VECTOR
252 C YP-USED BY CMBR FOR Y VECTOR
253 C
254 C
255 C CHARACTER TEST CONSTANTS
256 C BLANK,IBLANK-BLANK ' '
257 C ISTAR-PRINT FLAGS ' ' '*'
258 C QUOTA-'A' QUOTB-'B' QUOTC-'C' (COARSE, CODES)
259 C QUOTD-'D' (DONE)
260 C QUOTOL-'TOTAL' QUOTR-'R' (RECEPTOR)
261 C QUOTS-'S' (SOURCE, STOP) STAR-ASTERISK '*'
262 C YESY-'Y' (YES)
263 C
264 C *****
265 C
266 C
267 C
268 C
269 C SPECIFICATION AND DIMENSION
270 C
271 C REAL*8 COMAND(20),SIZNAM(3),SOUNAM(35),ELMENT(35),TEMPN,
272 C *COMND1,QUOTOL
273 C CHARACTER VARIABLES
274 C INTEGER*4 CHK,ELFT(35,2),SOFT(35,2),ANS,
275 C *YBACK(2),TYPE,YESY,
276 C * MFLAG(35,3),MFLAGB(35,3),DUM(20),ISTAR(3),
277 C * STAR,QUOTC,QUOTA,QUOTB,QUOTS,SPACE,CMBID(5),BACKID(5),
278 C * OLDID(5),QUOTR,QUOTD,TEMPID(6),LASTID(6),
279 C *SAVE(5), FLAG(8,3),YEAR,BYEAR,SITE(3),BSITE(3),DATE,BDATE
280 C
281 C NUMERIC VARIABLE SPECS
282 C INTEGER*4 ELHOLD(35,2),SOHOLD(35,2),
283 C *INITEL(21),INITSO(16),IMEL,IMSO,
284 C *MEL1(2),MSORC1(2), USTART,UDUR,
285 C *UNIT,NEL,NSOURC,MELMAX,MSOMAX,BSTART,BDUR,
286 C *IRTN,JRTN,IEL,JSOURC,NCMND,I,KEL,LEL, ICMND,UNIT6,UNIT10,UNIT13,
287 C *UNIT12,MEL,MSOURC,KSOURC,LSOURC,
288 C *EFVAR,SIZ,UNIT5,UNITX,UNIT9,

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

289      *SCODE(35),PCODE(35),ISHOLD(35),UNIT11,
290      *TEMPC, IFLAG(3),RIDGE
291  C
292  C
293      REAL*4 A(35,35,2),UA(35,35,2),SEL(2),USEL(2),
294      *USORC(35,3),UUSORC(35,3),UCNC(35,3),UUCNC(35,3),
295      *CLCN(35,3),UCLCN(35,3),UFMSS,UUFMSS,RATIO,URATIO,
296      *TX,UTX,X,UX,PCNT,UPCNT,UTMSS,UUTMSS,UCMSS,UUCMSS,
297      *BFMSS,UBFMSS,UBTMSS,BTMSS,BCMSS,UBCMSS,BCNC(35,3),UBCNC(35,3),
298      * SELK(35),UELK(35),VIFELK(35),SAINT(3),SET(3),USAINT(3)
299  C
300  C
301  C CHEMICAL ELEMENT BALANCE ARRAYS
302  C
303  C STORAGE FOR CMB SUBROUTINE (17 SOURCES, 21 SPECIES)
304  C THE INTERCEPT COUNTS AS A SOURCE
305      REAL F(21,17),C(21),V(21),SF(21,17), VK(31), W(21),
306      * YP(21),XP(21,17),XMEAN(17), XPX(17,17),
307      * XPXK(17,17),XPY(17),SX(17),S(17),TM(21),AP(17),SOLD(17),
308      * VIF(17),SAS(17,31),SAA(17,31),SSET(2)
309      INTEGER IS(17),IA(17),ITM(21),PNAM(17,6)
310      REAL*8 BLANK
311  C
312  C
313  C EQUIVALENCE STATEMENT
314      EQUIVALENCE (IS,S),(IA,AP),(ITM,TM)
315      EQUIVALENCE (IBLANK,BLANK),(STAR,ISTAR(2)),
316      * (XPXK,PNAM),
317      * (CMBID,SITE),(CMBID(4),YEAR),(CMBID(5),DATE),
318      * (BACKID,BSITE),(BACKID(4),BYEAR),(BACKID(5),BDATE)
319  C
320  C
321  C COMMON
322      COMMON /F/ PCODE,SCODE,NEL
323  C
324  C
325  C DATA STATEMENTS
326      DATA YBACK/'YES ','NO '/,YESY/'Y'/
327  C
328      DATA BLANK/' ',QUOTC,QUOTA,QUOTB,QUOTS/
329      * 'C','A','B','S'/,QUOTOL/'TOTAL'/,
330      * QUOTR,QUOTD/'R','D'/
331      DATA COMAND/
332      *'HELP ',
333      *'AE ', 'DE ', 'AS ', 'DS ', 'CMB ',
334      *'PSOLN ', 'PINFO ', 'PDATA ', 'WRITE ',
335      *'INITIAL ', 'PMATRIX ', 'PCOMP ', 'RESUME ',
336      *'AUTOFIT ', 'SELECT ', 'BACKOUT '

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

337 *'BACKIN ','EXIT ','SIZE '/'
338 C
339 DATA VK /0.0,0.005,0.01,0.015,0.020,0.025,
340 * 0.030,0.035,0.040,0.045,0.050, 0.060,0.070,0.080,0.090,
341 * 0.100, 0.12,0.14,0.16,0.18,0.20, 0.24,0.28,0.32,0.36,
342 * 0.40, 0.48,0.56,0.64,0.72,0.80 /
343 C
344 C
345 DATA SIZNAM/' FINE ','COARSE ','TOTAL '/'
346 C
347 DATA FLAG/' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',
348 * '--- ',' CEB',' MAT',' RIX ',' IS S',' INGU',' LAR ',' ---',
349 * '--- ',' NON',' CON',' VERG',' ENT ',' SOLU',' TION',' ---'/
350 DATA ISTAR/' ','*' ','** '/,NOSKIP/0/
351 C INITIALIZATION OF STARTING PARAMETERS
352 C SET OUTPUT UNIT NUMBERS
353 UNIT5=5
354 UNIT6=6
355 UNIT9=9
356 UNIT10=10
357 UNIT11=11
358 UNIT12=12
359 UNIT13=13
360 C MAXIMUM NUMBER OF FITTING ELEMENTS
361 MELMAX=21
362 C MAXIMUM NUMBER OF FITTING SOURCES
363 MSOMAX=17
364 MSOMIX=MSOMAX-1
365 C SET RETURN STATEMENT
366 IRTN=1
367 C NUMBER OF COMMANDS
368 NCMND=20
369 C DATA SEARCH CONTROL SET TO SELECT MODE
370 ICNTRL=4
371 C BACKGROUND SUBTRACT SET TO 'NONE'
372 IBACK=2
373 C
374 C
375 C - CREATE WORKING SOURCE MATRICES -
376 C
377 C CODE SOURCE NAMES AND POSITIONS FROM SONM FILE
378 110 NSOURC=0
379 DO 140 I=1,35
380 SOUNAM(I)=BLANK
381 SCODE(I)=0000
382 115 READ(2,120,ERR=130,END=150)TEMPC,TEMPN
383 120 FORMAT(I2,2X,A8)
384 SOUNAM(I)=TEMPN

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```
385      SCODE(I)=TEMPC
386      NSOURC=NSOURC+1
387      GO TO 140
388 C ERROR MESSAGE- FORMAT MISMATCH
389 130  WRITE(UNIT6,135)
390 135  FORMAT(1H , 'AN INPUT CARD DID NOT MATCH PROPER FORMAT' /
391      *1X, 'IN FILE SONM AND WAS IGNORED. CHECK THIS AT UPCOMING ' /
392      *1X, 'VERIFY POINT')
393      GO TO 115
394 140  CONTINUE
395 C CODE POLLUTANT NAMES AND POSITIONS FROM PONM FILE
396 150  NEL=0
397      KINDEX=0
398      DO 190 I=1,35
399      ELMENT(I)=BLANK
400      PCODE(I)=000
401 160  READ(3,170,ERR=180,END=200)TEMPC,TEMPN
402 170  FORMAT(I2,2X,A8)
403 C DO NOT CODE IF POLLUTANT IS MASS CONCENTRATION
404      IF(TEMPC.NE.01)GO TO 175
405      TEMPN=QUOTOL
406      KINDEX=1
407 175  ELMENT(I)=TEMPN
408      PCODE(I)=TEMPC
409      NEL =NEL+1
410      GO TO 190
411 C ERROR MESSAGE- FORMAT MISMATCH
412 180  WRITE(UNIT6,185)
413 185  FORMAT(1H , 'AN INPUT CARD DID NOT MATCH PROPER FORMAT' /
414      *1X, 'IN FILE PONM AND WAS IGNORED. CHECK THIS AT UPCOMING ' /
415      *1X, 'VERIFY POINT')
416      GO TO 160
417 190  CONTINUE
418 200  IF(KINDEX.EQ.1)GO TO 201
419      PCODE(I)=1
420      ELMENT(I)=QUOTOL
421      NEL=NEL+1
422 C INITIALIZE SOURCE MATRICES
423 201  DO 210 ISIZ=1,2
424      DO 210 I=1,NSOURC
425      DO 210 J=1,NEL
426      A(J,I,ISIZ)=0.000E-00
427      UA(J,I,ISIZ)=0.001E-02
428 210  CONTINUE
429 C CODE MATRICES
430      DO 270 ISIZ=1,2
431      IUNIT=ISIZ+6
432 215  READ(IUNIT,220,ERR=232,END=270)ISCODE,IPCODE,X,UX
```

TABLE CMB MAIN PROGRAM (CONTINUED)

```

433 220 FORMAT(I2,2X,I2,2X,F8.6,2X,F8.6)
434 IF(IPCODE.EQ.1)WRITE(UNIT6,221)IUNIT
435 221 FORMAT(' **WARNING** POLLUTANT CODE 1 IN DATA ON UNIT ',
436 * I2,/' CODE 1 IS RESERVED FOR TOTAL AEROSOL')
437 C MATCH SCODES
438 DO 230 J=1,NSOURC
439 IF(ISCODE.EQ.SCODE(J))GO TO 240
440 230 CONTINUE
441 C ERROR MESSAGE - NO SCODE MATCH
442 232 IF(ISIZ.EQ.1)WRITE(UNIT6,234)
443 234 FORMAT(1H,'FORMAT MISMATCH OR SOURCE CODE NOT IDENTIFIED FOR '/
444 *1X,'AN INPUT CARD IN SORF FILE . CARD IGNORED.')
445 WRITE(UNIT6,235)ISCODE
446 235 FORMAT(1X,'SOURCE CODE:',I3)
447 IF(ISIZ.EQ.2)WRITE(UNIT6,236)
448 236 FORMAT(1H,'FORMAT MISMATCH OR SOURCE CODE NOT IDENTIFIED FOR '/
449 *1X,'AN INPUT CARD IN SORC FILE . CARD IGNORED.')
450 GO TO 215
451 C MATCH PCODES
452 240 DO 250 K=1,NEL
453 IF(IPCODE.EQ.PCODE(K))GO TO 260
454 250 CONTINUE
455 C ERROR MESSAGE - NO MATCH
456 IF (ISIZ.EQ.1)WRITE(UNIT6,252)SOUNAM(J)
457 252 FORMAT(1H,'AN UNIDENTIFIED POLLUTANT CARD WAS FOUND IN'/
458 *1X,'FILE SORF , SOURCE-',A5)
459 IF(ISIZ.EQ.2)WRITE(UNIT6,254)SOUNAM(J)
460 254 FORMAT(1H,'AN UNIDENTIFIED POLLUTANT CARD WAS FOUND IN'/
461 *1X,'FILE SORC , SOURCE-',A5)
462 GO TO 215
463 260 A(K,J,ISIZ)=X
464 UA(K,J,ISIZ)=UX
465 GO TO 215
466 270 CONTINUE
467 C ADD TOTAL AEROSOL ELEMENT
468 DO 272 K=1,NEL
469 IF(PCODE(K).EQ.1) GO TO 273
470 272 CONTINUE
471 273 DO 274 ISIZ=1,2
472 DO 274 J=1,NSOURC
473 A(K,J,ISIZ)=1.0
474 UA(K,J,ISIZ)=0.000001
475 274 CONTINUE
476 C WRITE DATA TO SCREEN FOR INSPECTION
477 278 WRITE(UNIT6,300)
478 300 FORMAT(1X,'WOULD YOU LIKE TO LOOK AT THE SOURCE AND SPECIES '
479 *'LISTS?'
480 * ,/,2X,'TYPE YES OR NO.')
```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

481 301 READ(UNIT5,28001,ERR=278)ANS
482 302 FORMAT(A3)
483      IF(ANS .NE. YESY )GO TO 335
484      GO TO 304
485 304 WRITE(UNIT6,310)
486 310 FORMAT(1H , 'SOURCE SIGNATURE MATRICES ARE CODED AS FOLLOWS',/,
487      *1X, 'SOURCES:',/,
488      *1X, 'SOURCE #      SOURCE NAME',/ )
489      DO 315 I=1,NSOURC
490      WRITE(UNIT6,312)I,SOUNAM(I)
491 312 FORMAT(3X,I2,11X,A8)
492 315 CONTINUE
493      WRITE(UNIT6,320)
494 320 FORMAT(1H ,/,1X, 'SPECIES:',/,
495      *1X, 'SPECIES #      SPECIES NAME      ')
496      DO 330 I=1,NEL
497      WRITE(UNIT6,312)I,ELMENT(I)
498 330 CONTINUE
499 C
500 C
501 C
502 C
503 C      - SET UP INITIAL AUTOFIT POLLUTANTS AND SOURCES -
504 C
505 C
506 C
507 C  INITIALIZE FIT FLAGS
508      335 DO 340 IEL=1,NEL
509          ELHOLD(IEL,1)=0
510          INITEL(IEL)=0
511 340      ELFT(IEL,1)=IBLANK
512          DO 350 JSOURC=1,NSOURC
513              SOHOLD(JSOURC,1)=0
514              INITSO(JSOURC)=0
515 350      SOFT(JSOURC,1)=IBLANK
516 C  INPUT INITIAL AUTOFIT SOURCES AND ELEMENTS
517 360 WRITE(UNIT6,365)
518 365 FORMAT(1H , 'PLEASE INPUT INITIAL FITTING INFORMATION')
519      IMSO=0
520      DO 370 I=1,NSOURC
521 366 WRITE(UNIT6,367)I
522 367 FORMAT(1H0, 'INITIAL SOURCE ',I2,': XX')
523      READ(UNIT5,2420,ERR=366)INITSO(I),SPACE
524      IF (SPACE.EQ.IBLANK)INITSO(I)=INITSO(I)/10
525      IF(INITSO(I).EQ.0)GO TO 380
526      IF(INITSO(I).EQ.-1)GO TO 372
527      IMSO=IMSO+1
528 370 CONTINUE

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

529      GO TO 380
530      372 IMSO=MIN0(NSOURC,MSOMIX)
531      DO 373 I=1,NSOURC
532      373 INITSO(I)=I
533      380 WRITE(UNIT6,381)
534      381 FORMAT(' INITIAL SOURCES')
535      DO 390 I=1,IMSO
536      J=INITSO(I)
537      WRITE(UNIT6,425)J,SOUNAM(J)
538      390 CONTINUE
539      IMEL=0
540      WRITE(UNIT6,400)
541      400 FORMAT(' ',/,1X,'PLEASE INPUT SPECIES')
542      DO 410 I=1,NEL
543      403 WRITE(UNIT6,404)I
544      404 FORMAT(1H,'INITIAL SPECIES ',I2,': XX')
545      READ(UNIT5,2420,ERR=403)INITEL(I),SPACE
546      IF(SPACE.EQ.IBLANK)INITEL(I)=INITEL(I)/10
547      IF(INITEL(I).EQ.0)GO TO 420
548      IF(INITEL(I).EQ.-1)GO TO 411
549      IMEL=IMEL+1
550      410 CONTINUE
551      GO TO 420
552      411 IMEL=MIN0(NEL,MELMAX)
553      DO 412 I=1,IMEL
554      412 INITEL(I)=I
555      420 WRITE(UNIT6,421)
556      421 FORMAT(' INITIAL SPECIES')
557      DO 430 I=1,IMEL
558      J=INITEL(I)
559      WRITE(UNIT6,425)J,ELMENT(J)
560      425 FORMAT(' ',3X,I2,3X,A8)
561      430 CONTINUE
562      C OPERATOR DECISION- CORRECT INPUT OR CONTINUE
563      WRITE(UNIT6,435)
564      435 FORMAT(' ',/,1X,'ARE INITIAL SOURCES AND SPECIES CORRECT?')
565      READ(UNIT5,28001)CHK
566      IF(CHK.EQ.YESY)GO TO 441
567      WRITE(UNIT6,442)
568      442 FORMAT(' USE COMMANDS AE,DE,AS,DS FOR CHANGES.'/
569      * ' OR, DO YOU WANT A FRESH START?')
570      READ(UNIT5,28001)ANS
571      IF(ANS.EQ.YESY)GO TO 360
572      441 IRTN=0
573      SIZ=1
574      443 GO TO 4401
575      444 IF(SIZ.GE.2)GO TO 445
576      SIZ=2

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

577      GO TO 443
578      445 IRTN=1
579      WRITE(UNIT6,446)
580      446 FORMAT(' THE "HELP" COMMAND LISTS COMMANDS')
581      SIZ=1
582      WRITE(UNIT6,3110) SIZNAM(SIZ)
583      C
584      C
585      450 REWIND UNIT10
586      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
587      C
588      C
589      C
590      C
591      C      - START OF GENERAL INTERACTIVE NETWORK -
592      C
593      C
594      C
595      C      COMMAND SEQUENCE
596      490 WRITE(UNIT6,495)
597      495 FORMAT(1H ,'COMMAND NOT EXECUTED. TRY AGAIN')
598      500 WRITE(UNIT6,510)
599      510 FORMAT(1H ,'ENTER COMMAND')
600      READ(UNIT5,520,ERR=490)COMND1
601      520 FORMAT(A8)
602      DO 550 ICMND=1,NCMND
603      IF(COMND1.EQ.COMAND(ICMND))GO TO 600
604      550 CONTINUE
605      GO TO 490
606      C      BRANCHING
607      600 GO TO(
608      *1100,2400,2500,2600,2700,2800,
609      *42000,3000,3200,3400,4400,
610      *43000,52000,4000,
611      *4099,4200,4600,4700,5000,3100
612      *),ICMND
613      C
614      C
615      C
616      C      -HELP. LIST AND DEFINE AVAILABLE COMMANDS
617      1100 WRITE(UNIT6,1110)
618      1110 FORMAT(1H ,
619      *'HELP-LISTS THESE COMMANDS',/1H ,
620      *' ',/1H ,
621      *'---- DATA ACCESS AND SEQUENCING ----',/1H ,
622      *'AUTOFIT-SEQUENCES AUTOMATICALLY TO NEXT DATA SET',/1H ,
623      *'RESUME-RESUME AUTOFIT',/1H ,
624      *'SELECT-SELECT DATA SET FOR CMB',/1H ,

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

625      *'SIZE-CHANGE SIZE FRACTION'/' ' ,
626      *'EXIT-CLOSE FILES AND LEAVE',/1H ,
627      *' ',/1H ,
628      *'----- CMB OPERATIONS -----',/1H ,
629      *'AE-ADD A SPECIES TO THE FIT',/1H ,
630      *'DE-DELETE A SPECIES FROM THE FIT',/1H ,
631      *'AS-ADD A SOURCE TO THE FIT',/1H ,
632      *'DS-DELETE A SOURCE FROM THE FIT',/1H ,
633      *'CMB-PERFORM CMB:  OPTIONS ARE RIDGE & EFFECTIVE VARIANCE'/' ')
634      WRITE(UNIT6,1120)
635  1120  FORMAT(1H ,
636      *' ',/1H ,
637      *'----- SCREEN DISPLAY -----',/1H ,
638      *'PINFO-PRINT CURRENT STATUS ON SCREEN',/1H ,
639      *'PDATA-PRINT CURRENT CMB RESULTS ON SCREEN',/1H ,
640      *'PMATRIX-PRINT SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS,'/
641      * ' OR SOURCE AND SPECIES CODE LISTS'/' ' ,
642      *'PSOLN-PRINT ALL RIDGE SOLUTIONS',/' ' ,
643      *'PCOMP-PRINT COMPUTED AVERAGES OF CMB SERIES',/' ' ,
644      *' ',/1H ,
645      *'----- DATA STORAGE -----',/1H ,
646      *'WRITE-WRITE PRESENT CMB RESULTS TO FULL PRINTOUT',/1H ,
647      *'      SUMMARY,AND USER FOLLOWUP STORAGE FILES')
648      WRITE(UNIT6,1140)
649  1140  FORMAT(1H ,
650      *' ',/1H ,
651      *'----- BACKGROUND SITE OPERATIONS -----',/1H ,
652      *'BACKOUT-SELECT AND SUBTRACT A BACKGROUND DATA SET',/1H ,
653      *'BACKIN-ELIMINATE CURRENT BACKGROUND SUBTRACTION')
654      WRITE(UNIT6,1150)
655  1150  FORMAT('/', ' SELECT SHOULD NORMALLY BE THE FIRST COMMAND')
656      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
657  C
658  C
659  C
660  C
661  C      -AE.  ADD AN SPECIES TO THE FIT
662  2400  JRTN=1
663      WRITE(UNIT6,3110)SIZNAM(SIZ)
664      GO TO 2410
665  2405  WRITE(UNIT6,2407)
666  2407  FORMAT(1H , 'IMPROPER CODE, TRY AGAIN')
667  2410  WRITE(UNIT6,2415)
668  2415  FORMAT(1H , 'INPUT CODE OF ADDED SPECIES')
669      READ(UNIT5,2420,ERR=2405)IEL,SPACE
670  2417  IF(IEL.EQ.0)GO TO (500,2860,4120,4130,4132,4150,4250,4260,
671      *4270,4280),IRTN
672  2420  FORMAT( I2,T2,A1)

```

```

673      IF(SPACE.EQ.IBLANK)IEL=IEL/10
674      IF(IEL.LT.1.OR.IEL.GT.NEL)GO TO 2405
675 C CHECK TO SEE IF THIS IS ALREADY A FITTING SPECIES
676      IF(ELFT(IEL,SIZ).EQ.IBLANK)GO TO 2430
677      WRITE(UNIT6,2425)ELMENT(IEL)
678 2425  FORMAT(1H ,A8,' IS ALREADY A FITTING SPECIES')
679      GO TO (2410,2510,2610,2710,3402),JRTN
680 2430  IF(MEL1(SIZ).EQ.MELMAX)GO TO 2480
681      MEL1(SIZ)=MEL1(SIZ)+1
682      MEL=MEL1(SIZ)
683      ELFT(IEL,SIZ)=STAR
684      ELHOLD(MEL,SIZ)=IEL
685      GO TO (2410,2510,2610,2710,3402),JRTN
686 2480  WRITE(UNIT6,2490)MELMAX, ELMENT(IEL)
687 2490  FORMAT(1H , 'MAXIMUM OF ',I2,' FITTING SPECIES EXCEEDED. ',
688      :1X,A4,' NOT ADDED TO FIT')
689      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN *
690 C
691 C
692 C
693 C
694 C      -DE.  DELETE AN SPECIES FROM THE FIT
695 2500  JRTN=2
696      WRITE(UNIT6,3110)SIZNAM(SIZ)
697      GO TO 2510
698 2505  WRITE(UNIT6,2407)
699 2510  WRITE(UNIT6,2515)
700 2515  FORMAT(1H , 'INPUT CODE OF DELETED SPECIES')
701      READ(UNIT5,2420,ERR=2505)IEL,SPACE
702      IF(SPACE.EQ.IBLANK)IEL=IEL/10
703 2517  IF(IEL.EQ.0)GO TO (500,2860,4120,4130,4132,4150,4250,4260,
704      *4270,4280),IRTN
705      IF(IEL.LT.1.OR.IEL.GT.NEL)GO TO 2505
706 C CHECK TO SEE IF THIS IS A FITTING SPECIES ALREADY
707      IF(ELFT(IEL,SIZ).EQ.STAR)GO TO 2530
708 2523  WRITE(UNIT6,2525)ELMENT(IEL)
709 2525  FORMAT(1H ,A8,' IS NOT A FITTING SPECIES')
710      GO TO (2410,2510,2610,2710,3402),JRTN
711 2530  MEL=MEL1(SIZ)
712      DO 2540 KEL=1,MEL
713      IF(ELHOLD(KEL,SIZ).EQ.IEL)GO TO 2560
714 2540  CONTINUE
715      GO TO 2523
716 2560  MEL1(SIZ)=MEL1(SIZ)-1
717      MEL=MEL1(SIZ)
718      ELFT(IEL,SIZ)=IBLANK
719      DO 2570 LEL=KEL,MEL
720      ELHOLD(LEL,SIZ)=ELHOLD(LEL+1,SIZ)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

721 2570 CONTINUE
722      GO TO (2410,2510,2610,2710,3402),JRTN
723  C
724  C
725  C
726  C
727  C      -AS.  ADD A SOURCE TO THE FIT
728 2600  JRTN=3
729      WRITE(UNIT6,3110)SIZNAM(SIZ)
730      GO TO 2610
731 2605  WRITE(UNIT6,2407)
732 2610  WRITE(UNIT6,2615)
733 2615  FORMAT(1H , 'INPUT CODE OF ADDED SOURCE')
734      READ(UNIT5,2420,ERR=2605)JSOURC,SPACE
735      IF(SPACE.EQ.IBLANK)JSOURC=JSOURC/10
736 2617  IF(JSOURC.EQ.0)GO TO (500,2860,4120,4130,4132,4150,4250,4260,
737      *4270,4280),IRTN
738      IF(JSOURC.LT.1.OR.JSOURC.GT.NSOURC)GO TO 2605
739  C CHECK TO SEE IF THIS IS ALREADY A FITTING SOURCE
740      IF(SOFT(JSOURC,SIZ).EQ.IBLANK)GO TO 2630
741      WRITE(UNIT6,2625)SOUNAM(JSOURC)
742 2625  FORMAT(1H ,A8,' IS ALREADY A FITTING SOURCE')
743      GO TO (2410,2510,2610,2710,3402),JRTN
744 2630  IF(MSORC1(SIZ).EQ.MSOMAX)GO TO 2680
745      MSORC1(SIZ)=MSORC1(SIZ)+1
746      MSOURC=MSORC1(SIZ)
747      SOFT(JSOURC,SIZ)=STAR
748      SOHOLD(MSOURC,SIZ)=JSOURC
749      GO TO (2410,2510,2610,2710,3402),JRTN
750 2680  WRITE(UNIT6,2690)MSOMAX,SOUNAM(JSOURC)
751 2690  FORMAT(1H , 'MAXIMUM OF ',I2,' FITTING SOURCES EXCEEDED. ',
752      :1X,A8,' NOT ADDED TO FIT. ')
753      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
754  C
755  C
756  C
757  C
758  C      -DS.  DELETE A SOURCE FROM THE FIT
759 2700  JRTN=4
760      WRITE(UNIT6,3110)SIZNAM(SIZ)
761      GO TO 2710
762 2705  WRITE(UNIT6,2407)
763 2710  WRITE(UNIT6,2715)
764 2715  FORMAT(1H , 'INPUT CODE OF DELETED SOURCE')
765      READ(UNIT5,2420,ERR=2705)JSOURC,SPACE
766      IF(SPACE.EQ.IBLANK)JSOURC=JSOURC/10
767 2717  IF(JSOURC.EQ.0)GO TO (500,2860,4120,4130,4132,4150,4250,4260,
768      *4270,4280),IRTN

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

769      IF(JSOURC.LT.1.OR(JSOURC.GT.NSOURC)GO TO 2705
770  C   IS IT ALREADY A FITTING SOURC
771      IF(SOFT(JSOURC,SIZ).EQ.STAR)GO TO 2730
772  2723 WRITE(UNIT6,2725)SOUNAM(JSOURC)
773  2725 FORMAT(1H ,A8,' IS NOT A FITTING SOURCE')
774      GO TO (2410,2510,2610,2710,3402),JRTN
775  2730 MSOURC=MSORC1(SIZ)
776      DO 2740 KSOURC=1,MSOURC
777      IF(SOHOLD(KSOURC,SIZ).EQ(JSOURC)GO TO 2760
778  2740 CONTINUE
779      GO TO 2723
780  2760 MSORC1(SIZ)=MSORC1(SIZ)-1
781      MSOURC=MSORC1(SIZ)
782      SOFT(JSOURC,SIZ)=IBLANK
783      DO 2770 LSOURC=KSOURC,MSOURC
784      SOHOLD(LSOURC,SIZ)=SOHOLD(LSOURC+1,SIZ)
785  2770 CONTINUE
786      GO TO (2410,2510,2610,2710,3402),JRTN
787  C
788  C
789  C
790  C
791  C      -CMB. PERFORM CHEMICAL ELEMENT BALANCE
792  2800 NOSKIP=0
793  2801 IF(NOSKIP.EQ.1)GO TO 28032
794      WRITE(UNIT6,28000)
795  28000 FORMAT(' DO YOU WANT RIDGE SOLUTIONS?')
796      READ(UNIT5,28001)ANS
797  28001 FORMAT(A1)
798      IF(ANS.EQ.QUOTS)GO TO 28032
799      RIDGE=0
800      CWT=1.0
801      IF(ANS.NE.YESY) GO TO 28020
802      RIDGE=1
803      WRITE(UNIT6,28010)
804  28010 FORMAT(' CMB WILL SELECT THE BEST RIDGE SOLUTION'/
805      * ' DO YOU WANT TO SEE A SUMMARY OF THE OTHERS?')
806      READ(UNIT5,28001)ANS
807      IF(ANS.EQ.YESY)RIDGE=2
808      WRITE(UNIT6,28015)
809  28015 FORMAT(' IN THE SELECTION OF THE BEST RIDGE SOLUTION, '
810      * '/' WHAT WEIGHT DO YOU WANT? (DEFAULT=1.0)')
811      READ(UNIT5,28016)CWT0
812  28016 FORMAT(F10.0)
813      IF(CWT0.NE.0)CWT=CWT0
814      WRITE(UNIT6,28017)CWT
815  28017 FORMAT(' WEIGHT IS',F20.9)
816  28020 WRITE(UNIT6,28021)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

817 28021 FORMAT(' DO YOU WANT TO USE EFFECTIVE VARIANCES?')
818     EFVAR=0
819     READ(UNIT5,28001)ANS
820     IF(ANS.EQ.YESY)EFVAR=1
821 2820 CONTINUE
822     WRITE(UNIT6,28031)
823 28031 FORMAT(' DO YOU WANT TO INCLUDE THE INTERCEPT IN THE'
824 * ' MODEL?')
825     INTCEP=0
826     READ(UNIT5,28033)ANS,KBUG
827 28033 FORMAT(A1,2X,I1)
828     IF(ANS.NE.YESY) GO TO 28032
829     INTCEP=1
830     IF(MSOURC.LE.MSOMIX) GO TO 28032
831     WRITE(UNIT6,28034) MSOMAX
832 28034 FORMAT('/' NUMBER OF SOURCES PLUS INTERCEPT EXCEEDS ',I2)
833     GO TO 500
834 28032 CONTINUE
835 C ENCODE TRANSFER ARRAYS
836     MEL=MEL1(SIZ)
837     MSOURC=MSORC1(SIZ)
838     I=0
839     DO 2830 KEL=1,MEL
840     IEL=ELHOLD(KEL,SIZ)
841     C(KEL)=UCNC(IEI,SIZ)
842     V(KEL)=UUCNC(IEI,SIZ)
843     IF(V(KEL).GT. 0.0)GO TO 2824
844     IF(I.EQ.0)WRITE(UNIT6,2822)
845 2822 FORMAT(' **ERROR**      SOME RECEPTOR CONCENTRATION STANDARD ERRORS'
846 * ' ARE LESS THAN'/' OR EQUAL TO ZERO.      WEIGHTED REGRESSION '
847 * 'CANNOT BE DONE IN THIS CASE.')
848     WRITE(UNIT6,2823)IEL,ELMENT(IEI),UCNC(IEI,SIZ),UUCNC(IEI,SIZ)
849 2823 FORMAT(' ',I2,1X,A8,3X,'CONC=',F10.3,5X,'STD ERR=',F10.3)
850     I=1
851 2824 CONTINUE
852     DO 2825 KSOURC=1,MSOURC
853     JSOURC=SOHOLD(KSOURC,SIZ)
854     F(KEL,KSOURC)=A(IEI,JSOURC,SIZ)
855     SF(KEL,KSOURC)=UA(IEI,JSOURC,SIZ)
856 2825 CONTINUE
857 2830 CONTINUE
858     DO 2832 JSOURC=1,35
859     VIFELK(JSOURC)=0.0
860     SELK(JSOURC)=0.0
861     UELK(JSOURC)=0.0
862 2832 CONTINUE
863     IF(I.GT.0)GO TO 500
864     TOTALA=UCMSS

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

865      IF(SIZ.EQ.1)TOTALA=UFMSS
866      CALL CMBR(F,C,MEL,MSOURC,MELMAX,MSOMAX,SF,V,VK,TOTALA,SSET,
867      * KINDEX,SAS,SAA,SR2,R2LS,VIF,
868      * RIDGE,EFVAR,INTCEP,IERR,KBUG,CWT,
869      * W,XP,YP,XMEAN,XPX,XPXK,XPY,SX,S,TM,AP,SOLD,IS,IA,ITM
870      * )
871      IFLAG(SIZ)=IERR
872  C  INITIALIZE ALL SOURCES TO ZERO
873  2840  DO 2845 JSOURC=1,NSOURC
874      USORC(JSOURC,SIZ)=0.0
875      UUSORC(JSOURC,SIZ)=0.0
876  2845  CONTINUE
877  C  REPLACE SOURCES WITH CALCULATED VALUES
878  2850  CONTINUE
879      SETLS=SSET(1)
880      SET(SIZ)=SSET(2)
881      DO 2855 KSOURC=1,MSOURC
882      JSOURC=SOHOLD(KSOURC,SIZ)
883      USORC(JSOURC,SIZ)=SAS(KSOURC,KINDEX)
884      UUSORC(JSOURC,SIZ)=SAA(KSOURC,KINDEX)
885      VIFELK(JSOURC)=VIF(KSOURC)
886      SELK(JSOURC)=SAS(KSOURC,1)
887      UELK(JSOURC)=SAA(KSOURC,1)
888  2855  CONTINUE
889      IF(INTCEP.EQ.0)GO TO 2856
890      I=MSOURC+1
891      SAINT(SIZ)=SAS(I,KINDEX)
892      USAINT(SIZ)=SAA(I,KINDEX)
893      SAINTO=SAS(I,1)
894      USAINO=SAA(I,1)
895      GO TO 2857
896  2856  SAINT(SIZ)=0.0
897      SAINTO=0.0
898      USAINT(SIZ)=0.0
899      USAINO=0.0
900  C  GO TO CALCON
901  2857  IRTN=2
902      GO TO 3800
903  2860  IRTN=1
904  C  PRINT ON SCREEN
905  C  NO SOLUTION DISPLAYED FOR SINGULAR MATRIX
906      IF(IERR.EQ.1)GO TO 500
907      GO TO 3200
908  C
909  C
910  C
911  C
912  COMMAND  -PSOLN.  PRINT ALL RIDGE SOLUTIONS ON SCREEN

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

913 C OR HARD COPY
914 C
915 42000 CONTINUE
916 IF(RIDGE.EQ.0)GO TO 42060
917 J=31*(2*MSOURC+1)
918 I=MSOURC+1
919 WRITE(UNIT6,42001) MSOURC,J
920 42001 FORMAT(' THERE ARE 31 SOLUTIONS WITH AN INTERCEPT'/
921 * ' AND ',I2,' SOURCE COEFICIENTS AND STANDARD ERRORS'/
922 * ' EACH FOR ',I4,' NUMBERS TOTAL.'/
923 * ' THEY CAN PRINT TO YOUR TERMINAL OR TO HARD COPY.'/
924 * ' ARE YOU SURE YOU WANT TO LOOK AT THESE NUMBERS?')
925 READ(UNIT5,28001)ANS
926 IF (ANS.NE.YESY) GO TO 500
927 WRITE(UNIT6,42002)
928 42002 FORMAT(' DO YOU WANT THE SOLUTIONS PRINTED ON THE HARD COPY',
929 * / ' (INSTEAD OF AT YOUR TERMINAL)?')
930 READ(UNIT5,28001)ANS
931 UNITX=UNIT6
932 MANY=2
933 IF(ANS.NE.YESY)GO TO 42004
934 UNITX=UNIT11
935 MANY=6
936 GO TO 42005
937 42004 WRITE(UNIT6,42010)
938 42010 FORMAT(' CAN YOUR TERMINAL DISPLAY A 132 CHARACTER LINE?')
939 READ(UNIT5,28001)ANS
940 IF(ANS.EQ.YESY)MANY=6
941 42005 MORE=MANY+1
942 IF(INTCEP.EQ.0)WRITE(UNIT6,42011)
943 42011 FORMAT('/' ZERO INTERCEPT IN MODEL'/)
944 DO 42050 KEL=1,31,MORE
945 IEL=KEL+MANY
946 IF(IEL.GT.31)IEL=31
947 WRITE(UNITX,42006)(VK(J),J=KEL,IEL)
948 IF(INTCEP.GT.0)
949 *WRITE(UNITX,42007)(SAS(I,J),SAA(I,J),J=KEL,IEL)
950 42006 FORMAT('/' RIDGE K',5X,7(F7.3,10X))
951 42007 FORMAT(' INTERCEPT',3X, 7(F7.3,'+-',F6.3,2X))
952 DO 42040 KSOURC=1,MSOURC
953 JSOURC=SOHOLD(KSOURC,SIZ)
954 WRITE(UNITX,42008) SOUNAM(JSOURC),(SAS(KSOURC,J),
955 * SAA(KSOURC,J),J=KEL,IEL)
956 42008 FORMAT(' ',A8,4X,7(F7.3,'+-',F6.3,2X))
957 42040 CONTINUE
958 42050 CONTINUE
959 IF (UNITX.EQ.UNIT11 ) WRITE(UNIT6,42051)
960 42051 FORMAT(' SOLUTIONS WRITTEN TO HARD COPY')

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

961      GO TO 500
962 42060 WRITE(UNIT6,42061)
963 42061 FORMAT(' THE RIDGE OPTION WAS NOT USED - ONLY 1 SOLUTION')
964      GO TO 500
965 C
966 C
967 COMMAND      -PMATRIX      PRINT SOURCE SIGNATURE MATRIX, RECEPTOR
968 C                      RECEPTOR CONCENTRATIONS
969 C                      CODES FOR SOURCES AND SPECIES
970 C
971 43000 CONTINUE
972 C
973      LOOP=0
974      UNITX=UNIT11
975      WRITE(UNIT6,43002)
976 43002 FORMAT(' MATRICES CAN GO TO HARD COPY'/
977      * ' DO YOU WANT THEM DISPLAYED AT YOUR TERMINAL INSTEAD?')
978      READ(UNIT5,28001) ANS
979      IF(ANS.EQ.YESY)UNITX=UNIT6
980 43005 WRITE(UNIT6,43010)
981 43010 FORMAT(' WHAT DO YOU WANT TO SEE?'/
982      * ' SOURCE SIGNATURE, RECEPTOR CONCENTRATIONS, OR CODES?')
983      IF(LOOP.EQ.1)WRITE(UNIT6,43020)
984 43020 FORMAT(' OR ARE YOU DONE?')
985      READ(UNIT5,28001,ERR=43005) ANS
986      IF (ANS.EQ.QUOTD .OR. ANS.EQ.YESY .OR. ANS.EQ.IBLANK)
987      * GO TO 500
988      LOOP=1
989      IF(ANS.EQ.QUOTR)GO TO 3700
990      IF(ANS.EQ.QUOTS)GO TO 43039
991      IF(ANS.EQ.QUOTC)GO TO 43800
992      WRITE(UNIT6,43060)
993 43060 FORMAT(' INVALID REQUEST')
994      GO TO 43005
995 43039 CONTINUE
996      WRITE(UNIT6,43040)
997 43040 FORMAT(' WHAT SIZE FRACTION? (FINE OR COARSE)')
998      READ(UNIT5,28001)CHK
999      ISIZ=1
1000      IF(CHK.EQ.QUOTC) ISIZ=2
1001 43310 FORMAT(' ',I2,1X,A8,5X,F8.4,2X,'+-',2X,F8.4)
1002 C DISPLAY SOURCE SIGNATURE
1003 43200 CONTINUE
1004      WRITE(UNIT6,43210) NSOURC,NEL
1005 43210 FORMAT(' DO YOU WANT TO LOOK AT THE WHOLE MATRIX?'/
1006      * ' IT IS ',I2,' SOURCES BY ',I2,' SPECIES')
1007      READ(UNIT5,28001)ANS
1008      IF(ANS.NE.YESY) GO TO 43500

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1009 C DISPLAY WHOLE SOURCE SIGNATURE MATRIX
1010     IWIDE=1
1011     IF(UNITX.NE.UNIT6)GO TO 43213
1012     WRITE(UNIT6,43045)
1013 43045 FORMAT(' CAN YOUR TERMINAL DISPLAY A 132 CHARACTER LINE?')
1014     READ(UNIT5,28001)ANS
1015     IF(ANS.NE.YESY)IWIDE=0
1016 43213 MANY=5
1017     IF(IWIDE.EQ.1)MANY=12
1018     MORE=MANY+1
1019     DO 43240 KEL=1,NSOURC,MORE
1020     IEL=KEL+MANY
1021     IF(IEL.GT.NSOURC)IEL=NSOURC
1022     WRITE(UNITX,43218)(SOUNAM(I),I=KEL,IEL)
1023 43218 FORMAT(' ',14X,13A9)
1024     DO 43230 J=1,NEL
1025     WRITE(UNITX,43220)J, ELEMENT(J),(A(J,I,ISIZ),I=KEL,IEL)
1026     WRITE(UNITX,43221) (UA(J,I,ISIZ),I=KEL,IEL)
1027 43220 FORMAT(/' ',I2,1X,A8,3X,13F9.4)
1028 43221 FORMAT(' ',14X,13F9.4)
1029 43230 CONTINUE
1030 43240 CONTINUE
1031     GO TO 43005
1032 C DISPLAY INDIVIDUAL SOURCE SIGNATURES
1033 43500 CONTINUE
1034 43502 WRITE(UNIT6,43510)
1035 43510 FORMAT(' WHICH SOURCE DO YOU WANT?'/
1036     * ' GIVE SOURCE #')
1037     READ(UNIT5,2420,ERR=43502)I,SPACE
1038     IF(SPACE.EQ.IBLANK)I=I/10
1039     IF(I.LE.0)GO TO 43005
1040     WRITE(UNITX,43515) SOUNAM(I)
1041 43515 FORMAT(' SOURCE: ',A8)
1042     DO 43520 J=1,NEL
1043     WRITE(UNITX,43310) J,ELEMENT(J),A(J,I,ISIZ),UA(J,I,ISIZ)
1044 C DISPLAY SOURCES AND SPECIES CODE LISTS
1045 43520 CONTINUE
1046     GO TO 43500
1047 43800 CONTINUE
1048     WRITE(UNITX,43810)
1049 43810 FORMAT(/' SOURCE #',8X,'NAME',12X,'CODE')
1050     DO 43820 I=1,NSOURC
1051     WRITE(UNITX,43815) I,SOUNAM(I),SCODE(I)
1052 43815 FORMAT(' ',3X,I2,10X,A8,10X,I2)
1053 43820 CONTINUE
1054     WRITE(UNITX,43830)
1055 43830 FORMAT(/' SPECIES #',7X,'NAME',12X,'CODE')
1056     DO 43840 I=1,NEL

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1057      WRITE(UNITX,43815)I,ELMENT(I),PCODE(I)
1058 43840 CONTINUE
1059      WRITE(UNITX,43850)
1060 43850 FORMAT(/' USE SOURCE # AND SPECIES # FOR ALL YOUR '
1061      * 'RESPONSES'/' USE CODES ONLY WHEN CODING '
1062      * 'MATRICES FOR THE DATA BASE')
1063      GO TO 43005
1064 C
1065 C
1066 C
1067 C      -PINFO.  PRINT CURRENT STATUS ON SCREEN
1068 3000  WRITE(UNIT6,3005)
1069 3005  FORMAT('          ***CURRENT STATUS***')
1070      WRITE(UNIT6,3030)CMBID,SIZNAM(SIZ),UDUR,USTART,YBACK(IBACK)
1071 3030  FORMAT(' CMB SITE: ',3A4,5X,'YEAR: ',A2,3X,'DATE: ',A4/
1072      * 1X,A8,'SIZE FRACTION'/
1073      * 1X,'DURATION: ',I2,' START HOUR: ',I2,/,
1074      * 1X,'HAS BACKGROUND BEEN SUBTRACTED: ',A3)
1075      IF(IBACK.EQ.2)GO TO 3040
1076      WRITE(UNIT6,3035)BACKID,BDUR,BSTART
1077 3035  FORMAT(1H , 'SUBTRACTED BACKGROUND CMB SITE: ',3A4,5X,
1078      * 'YEAR: ',A2,3X,'DATE: ',A4/
1079      * 1X,'DURATION: ',I2,' START HOUR: ',I2)
1080 3040  WRITE(UNIT6,3045)
1081 3045  FORMAT(1H , 'FITTING SPECIES')
1082      DO 3055 KEL=1,MEL
1083      IEL=ELHOLD(KEL,SIZ)
1084      WRITE(UNIT6,425)IEL,ELMENT(IEL)
1085 3055  CONTINUE
1086      WRITE(UNIT6,3060)
1087 3060  FORMAT(1H , 'FITTING SOURCES')
1088      DO 3080 KSOURC=1,MSOURC
1089      JSOURC=SOHOLD(KSOURC,SIZ)
1090      WRITE(UNIT6,425)JSOURC,SOUNAM(JSOURC)
1091 3080  CONTINUE
1092      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1093 C
1094 C
1095 C
1096 C      -SIZE.  CHANGES SIZE FRACTION BETWEEN FINE AND COARSE
1097 C
1098 C
1099 C
1100 3100  ISIZ=SIZ
1101      IF(ISIZ.EQ.1)SIZ=2
1102      IF(ISIZ.EQ.2)SIZ=1
1103      WRITE(UNIT6,3110)SIZNAM(SIZ)
1104 3110  FORMAT(' SIZE IS ',A8)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1105      IRTN=1
1106      GO TO 500
1107  C
1108  C
1109  C
1110  C
1111  C      -PDATA.  PRINTS CURRENT CMB RESULTS TO SCREEN
1112  C
1113  C
1114      3200 I=2-EFVAR
1115          WRITE(UNIT6,3205)CMBID,SIZNAM(SIZ),UDUR,USTART,YBACK(IBACK),
1116          * YBACK(I),SR2,VK(KINDEX),R2LS
1117      3205 FORMAT('0CMB SITE: ',3A4,5X,'YEAR: ',A2,3X,'DATE: ',A4,6X,
1118          * 'FRACTION: ',A6/ ' SAMPLE DURATION: ',I2,
1119          * ' WITH START HOUR: ',I2,2X,'BACKGROUND: ',A3,
1120          * 2X,'EFF VAR: ',A3/
1121          * 1X,9('-'),'RIDGE REGRESSION',8('-'),4X,5('-'),
1122          * 'WEIGHTED LEAST SQUARES',5('-')/
1123          * 3X,'R-SQUARE:',F6.4,3X,'RIDGE K=',F5.3,12X,
1124          * 'R-SQUARE:',F6.4/
1125          * ' ---SOURCE',10('-'),'UG/M3',9('-'),4X,7('-'),'UG/M3',
1126          * 10('-'),'VIF',7('-'))
1127          WRITE(UNIT6,3208)SAINT(SIZ),USAINT(SIZ),SAINTO,USAINO
1128      3208  FORMAT(3X,'INTERCEPT',F10.3,'+-',F8.3,5X,F10.3,'+-',F8.3)
1129          X=SAINT(SIZ)
1130          XX=SAINTO
1131          DO 3240 JSOURC=1,NSOURC
1132          IF(UUSORC(JSOURC,SIZ).LE.0.)GO TO 3240
1133          WRITE(UNIT6,3230)JSOURC,SOUNAM(JSOURC),
1134          1USORC(JSOURC,SIZ),UUSORC(JSOURC,SIZ),SELK(JSOURC),UELK(JSOURC),
1135          * VIFELK(JSOURC)
1136      3230  FORMAT(1H ,I2,1X,A8,F10.3,'+-',F8.3,
1137          * 5X,F10.3,'+-',F8.3,1X,F8.3)
1138          X=X+USORC(JSOURC,SIZ)
1139          XX=XX+SELK(JSOURC)
1140      3240  CONTINUE
1141          WRITE(UNIT6,3245)X,SET(SIZ),XX,SETLS
1142      3245  FORMAT(1H , 'TOTAL: ',4X,F10.3,'+-',F8.3,5X,F10.3,'+-',F8.3)
1143          WRITE(UNIT6,3279)
1144          WRITE(UNIT6,3280)UFMSS,UUFMSS,UCMSS,UUCMSS,UTMSS,UUTMSS
1145      3279  FORMAT(1H , 'MEASURED CONCENTRATION FINE/COARSE/TOTAL:')
1146      3280  FORMAT(1H ,2(F10.5,'+-',F8.3,'/'),F10.5,'+-',F8.3)
1147      3241  WRITE(UNIT6,3250)
1148      3250  FORMAT(1X,'PRESS RETURN TO CONTINUE OR ENTER C FOR NEXT ',
1149          * 'COMMAND')
1150      3243  READ(UNIT5,28001,ERR=3248)ANS
1151          IF(ANS .EQ. QUOTC)GO TO 3275
1152          IF(ANS .EQ. IBLANK)GO TO 3244

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1153 C  OPTION TO "STOP" IN AUTOFIT
1154     IF(ANS .NE. QUOTS)GO TO 3248
1155     3246 IRTN=1
1156         KCNTRL=ICNTRL
1157         ICNTRL=4
1158         GO TO 500
1159     3248 WRITE(UNIT6,3249)
1160     3249 FORMAT(1X,'INPUT ERROR.')
1161         GO TO 3241
1162     3244 WRITE(UNIT6,3247)
1163     3247 FORMAT(1H ,25('-'),'MEAS',12('-'),'CALC',10('-'),'RATIO',10('-'))
1164 CORRECT STD. ERR. FOR TOTAL AEROSOL
1165     UCLCN(1,SIZ)=SET(SIZ)
1166     DO 3270 IEL=1,NEL
1167         IF(UCNC(IEL,SIZ).LE.0.)RATIO=0.
1168         IF(UCNC(IEL,SIZ).LE.0.)URATIO=0.
1169         IF(UCNC(IEL,SIZ).LE.0)GO TO 3242
1170         RATIO=CLCN(IEL,SIZ)/UCNC(IEL,SIZ)
1171         URATIO=((UCLCN(IEL,SIZ)/UCNC(IEL,SIZ))**2+(UUCNC(IEL,SIZ)
1172     1*CLCN(IEL,SIZ)/UCNC(IEL,SIZ)**2)**2)**.5
1173     3242 IF(UCNC(IEL,SIZ).GE.UUCNC(IEL,SIZ))
1174         1WRITE(UNIT6,3260)IEL,ELMENT(IEL),ELFT(IEL,SIZ),MFLAG(IEL,SIZ),
1175         1UCNC(IEL,SIZ),
1176         1UUCNC(IEL,SIZ),CLCN(IEL,SIZ),UCLCN(IEL,SIZ),RATIO,URATIO,
1177         1ELMENT(IEL)
1178         IF(UCNC(IEL,SIZ).LT.UUCNC(IEL,SIZ))
1179         1WRITE(UNIT6,3265)IEL,ELMENT(IEL),ELFT(IEL,SIZ),MFLAG(IEL,SIZ),
1180         1UUCNC(IEL,SIZ),CLCN(IEL,SIZ),UCLCN(IEL,SIZ),
1181         1RATIO,URATIO,ELMENT(IEL)
1182     3260 FORMAT(1H ,I2,1X,A8,2X,A1,2X,A1,1X,F7.3,'+-',F6.3,1X,
1183     11X,F7.3,'+-',F6.3,1X,F5.2,'+-',F5.2,2X,A3)
1184     3265 FORMAT(1H ,I2,1X,A8,2X,A1,2X,A1,1X,7X,'< ',F6.3,1X,
1185     11X,F7.3,'+-',F6.3,1X,F5.2,'+-',F5.2,2X,A3)
1186     3270 CONTINUE
1187 CHANCE TO HOLD FOR CRT
1188     IF(ICNTRL.NE.2 .AND. ICNTRL.NE.0)GO TO 3276
1189     IRTN=5
1190     IF(SIZ.EQ.2 .AND. ICNTRL.EQ.0)GO TO 3276
1191     READ(UNIT5,28001)ANS
1192     IF(ANS.EQ.QUOTS)GO TO 3246
1193     GO TO 3276
1194     3275 IF(ICNTRL.EQ.2 .OR. ICNTRL.EQ.0)IRTN=5
1195     3276 GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1196 C
1197 C
1198 C
1199 C
1200 C      -WRITE.  WRITES DATA TO HARDCOPY

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1201 3400 JRTN=5
1202 C
1203 3402 UNIT=UNIT11
1204 ISIZ=SIIZ
1205 IPF=IFLAG(ISIZ)
1206 3413 WRITE(UNIT,3415)CMBID,(FLAG(I,IPF+1),I=1,8),SIIZNAM(ISIZ)
1207 3415 FORMAT(' ',/,1X,'RESULTS FOR CMB SITE: ',3A4,5X,
1208 * 'YEAR: ',A2,3X,'DATE: ',A4,4X,8A4,
1209 * 1X,/,', ',A6,', PARTICULATE FRACTION')
1210 3417 FORMAT(1X,', ')
1211 WRITE(UNIT,3430)UDUR,USTART
1212 3430 FORMAT(
1213 * 1X,'SAMPLING DURATION: ',I2,', HRS. WITH START HOUR: ',I2)
1214 WRITE(UNIT,3440)YBACK(IBACK)
1215 3440 FORMAT(1H,'BACKGROUND SITE SUBTRACTED: ',A3)
1216 IF(IBACK.EQ.2)GO TO 3460
1217 C WRITE BACKG INFO
1218 WRITE(UNIT,3450)BACKID
1219 3450 FORMAT(' BACKGROUND CMB SITE: ',3A4,5X,
1220 * 'YEAR: ',A2,3X,'DATE: ',A4)
1221 WRITE(UNIT,3430)BDUR,BSTART
1222 3460 IF(ISIZ.NE.3)GO TO 3466
1223 WRITE(UNIT,3468)
1224 3468 FORMAT(' RESULTS DERIVED FROM FINE AND COARSE FITTINGS')
1225 SAINT(3)=SAINT(1)+SAINT(2)
1226 USAINT(3)=SQRT(USAINT(1)**2+USAINT(2)**2)
1227 WRITE(UNIT,3477)SAINT(3),USAINT(3)
1228 GO TO 3478
1229 3466 IF(INTCEP.EQ.0)WRITE(UNIT,3469)
1230 3469 FORMAT(' INTERCEPT SET TO ZERO')
1231 IF(RIDGE.EQ.0)WRITE(UNIT,3470)
1232 3470 FORMAT(' RIDGE OPTION NOT USED')
1233 IF(EFVAR.GT.0)WRITE(UNIT,3471)
1234 3471 FORMAT(' EFFECTIVE VARIANCE METHOD')
1235 C WRITE HEADER
1236 3474 WRITE(UNIT,3476)VK(KINDEX),SR2,R2LS,SAINT(ISIZ),USAINT(ISIZ),
1237 * SAINTO,USAINO
1238 3476 FORMAT(25X,'RIDGE REGRESSION',25X,'LEAST SQUARES'/
1239 * 25X,'K=',F5.3,5X,'R-SQUARE: ',F6.4,13X,'K=0.0',5X,
1240 * 'R-SQUARE: ',F6.4/,', ',120('-',')/
1241 * 1X,'CODE',2X,'SOURCE',13X,'UG/M3',15X,'% ',
1242 * 22X,'UG/M3',13X,'VIF'/', ',120('-',')
1243 * /5X,'INTERCEPT',3X,F8.3,'+-',F8.3,26X,F8.3,'+-',F8.3)
1244 3477 FORMAT(/', ',120('-',')/1X,'CODE',2X,'SOURCE',13X,'UG/M3',
1245 * 15X,'% '/', ',120('-',')/5X,'INTERCEPT',3X,F8.3,'+-',F8.3)
1246 C WRITE SOURCES
1247 3478 TX=SAINT(ISIZ)
1248 XX=SAINTO

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1249      ISCTR=0
1250      DO 3490 JSOURC=1,NSOURC
1251      IF(UUSORC(JSOURC,1).LE.0..AND.UUSORC(JSOURC,2)
1252      1.LE.0.)GO TO 3490
1253      IF(ISIZ.EQ.1.AND.UUSORC(JSOURC,1).LE.0.)GO TO 3490
1254      IF(ISIZ.EQ.1)X=UFMSS
1255      IF(ISIZ.EQ.1)UX=UUFMSS
1256      IF(ISIZ.EQ.2)X=UCMSS
1257      IF(ISIZ.EQ.2)UX=UUCMSS
1258      IF(ISIZ.EQ.3)X=UTMSS
1259      IF(ISIZ.EQ.3)UX=UTMSS
1260  C   GET TOTAL SOURCE
1261      IF(ISIZ.NE.3)GO TO 3480
1262      USORC(JSOURC,3)=USORC(JSOURC,1)+USORC(JSOURC,2)
1263      UUSORC(JSOURC,3)=((UUSORC(JSOURC,1))*2+UUSORC(JSOURC,2))*2)**.5
1264 3480  CALL PERC(PCNT,UPCNT,USORC(JSOURC,ISIZ),UUSORC(JSOURC,ISIZ),X,UX)
1265      IF(UX.LE.0.)GO TO 3490
1266      IF(ISIZ.LT.3)WRITE(UNIT,3485)JSOURC,SOUNAM(JSOURC),
1267      1USORC(JSOURC,ISIZ),UUSORC(JSOURC,ISIZ),PCNT,UPCNT,
1268      *   SELK(JSOURC),UELK(JSOURC),VIFELK(JSOURC)
1269      IF(ISIZ.EQ.3) WRITE(UNIT,3485) JSOURC,SOUNAM(JSOURC),
1270      *   USORC(JSOURC,ISIZ),UUSORC(JSOURC,ISIZ),PCNT,UPCNT
1271 3485  FORMAT(1X,I2,3X,A8,1X,F10.3,'+-',F8.3,2X,F7.3,'+-',F6.3,
1272      *   7X,F10.3,'+-',F8.3,2X,F8.3)
1273      TX=TX+USORC(JSOURC,ISIZ)
1274      XX=XX+SELK(JSOURC)
1275  C   INCREMENT SOURCE COUNTER
1276      ISCTR=ISCTR+1
1277  C   IF TOTAL FRACTION, HOLD SOURCE CODES FOR SUMMARY
1278      IF (ISIZ.EQ.3)ISHOLD(ISCTR)=JSOURC
1279 3490  CONTINUE
1280      IF(ISIZ.EQ.3)SET(3)=SQRT(SET(1)**2+SET(2)**2)
1281      WRITE(UNIT,3499)
1282      CALL PERC(PCNT,UPCNT,TX,SET(ISIZ),X,UX)
1283      IF(ISIZ.LT.3)WRITE(UNIT,3491)TX,SET(ISIZ),PCNT,UPCNT,XX,SETLS
1284      IF(ISIZ.EQ.3)WRITE(UNIT,3491)TX,SET(ISIZ),PCNT,UPCNT
1285 3491  FORMAT(6X,'TOTAL:',3X,F10.3,'+-',F8.3,2X,F7.3,'+-',F6.3,7X,F10.3,
1286      *   '+-',F8.3)
1287      WRITE(UNIT,3417)
1288  C   WRITE ELEMENTS
1289  C   WRITE HEADER
1290      WRITE(UNIT,3495)SIZNAM(ISIZ)
1291 3495  FORMAT(1X,'SPECIES      FIT',2X,'MISS',9X,A6,1X,
1292      *   'SUSPENDED PARTICULATE')
1293      WRITE(UNIT,3497)
1294 3497  FORMAT(' CODE          FLG',2X,'FLG',3X,'MEAS. UG/M3',8X,
1295      *   1X,'PERCENT',7X,'CALC. UG/M3',7X,'RATIO')
1296      WRITE(UNIT,3499)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1297 3499 FORMAT(1X,120('-'))
1298 3500 FORMAT(2X,I2,2X,A6,2X,A1,2X,A1,2X,2(F7.3,'+-',F6.3,1X),1X,
1299 11X,F7.3,'+-',F6.3,1X,F6.3,'+-',F6.3,2X,A8)
1300 3505 FORMAT(2X,I2,2X,A6,2X,A1,2X,A1,2X,2(7X,'< ',F6.3,1X),
1301 12X,F7.3,'+-',F6.3,1X,F6.3,'+-',F6.3,2X,A8)
1302 CORRECT STD. ERR. FOR TOTAL
1303 UCLCN(1,ISIZ)=SET(ISIZ)
1304 DO 3530 IEL=1,NEL
1305 IF(ISIZ.EQ.3)CLCN(1,ISIZ)=CLCN(1,1)+CLCN(1,2)
1306 IF(ISIZ.EQ.3)UCLCN(1,ISIZ)=
1307 *SQRT((UCLCN(1,1))**2+(UCLCN(1,2))**2)
1308 3525 IF(UCNC(1,ISIZ).EQ.0.)RATIO=0.
1309 IF(UCNC(1,ISIZ).LE.0.)URATIO=0.
1310 IF(UCNC(1,ISIZ).LE.0.)GO TO 3526
1311 RATIO=CLCN(1,ISIZ)/UCNC(1,ISIZ)
1312 URATIO=SQRT((UCLCN(1,ISIZ)/UCNC(1,ISIZ))**2+
1313 *(UCLCN(1,ISIZ)*CLCN(1,ISIZ)/UCNC(1,ISIZ)**2)**2)
1314 3526 CALL PERC(PCNT,UPCNT,UCNC(1,ISIZ),UUCNC(1,ISIZ),X,UX)
1315 IF(UCNC(1,ISIZ).GE.UUCNC(1,ISIZ))WRITE(UNIT,3500)IEL,
1316 *ELEMENT(1),ELFT(1,ISIZ),MFLAG(1,ISIZ),UCNC(1,ISIZ),UUCNC
1317 *(1,ISIZ),PCNT,UPCNT,CLCN(1,ISIZ),UCLCN(1,ISIZ),RATIO,URATIO,
1318 *ELEMENT(1)
1319 IF(UCNC(1,ISIZ).LT.UUCNC(1,ISIZ))WRITE(UNIT,3505)IEL,
1320 *ELEMENT(1),ELFT(1,ISIZ),MFLAG(1,ISIZ),UCNC(1,ISIZ),UPCNT,
1321 *CLCN(1,ISIZ),UCLCN(1,ISIZ),RATIO,URATIO,ELEMENT(1)
1322 3530 CONTINUE
1323 WRITE(UNIT,3499)
1324 C WRITE MASSES
1325 WRITE(UNIT,3540)UFMSS,UUFMSS,UCMSS,UUCMSS,UTMSS,UUTMSS
1326 3540 FORMAT(' MEASURED AMBIENT MASS (UG/M3): FINE: ',
1327 *1X,F5.1,'+-',F4.1,' COARSE: ',F5.1,'+-',F4.1,' TOTAL: ',
1328 *1X,F5.1,'+-',F4.1)
1329 WRITE(UNIT,3543)
1330 3543 FORMAT(////'1')
1331 3545 WRITE(UNIT6,3546)
1332 3546 FORMAT(' WRITTEN')
1333 IF(ISIZ.NE.1)GO TO 3549
1334 DO 3547 IEL=1,5
1335 3547 OLDDID(1)=CMBID(1)
1336 3548 GO TO (500,2860,4120,4130,4132,4150,4250,4260,
1337 *4270,4280),IRTN
1338 3549 IF(ISIZ.EQ.3)GO TO 3600
1339 3550 DO 3552 IEL=1,5
1340 IF(OLDDID(1).NE.CMBID(1))GO TO 3548
1341 3552 CONTINUE
1342 ISIZ=3
1343 IPF=0
1344 IF(IFLAG(1).EQ.2.OR.IFLAG(2).EQ.2)IPF=2

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1345      IF(IFLAG(1).EQ.1.OR.IFLAG(2).EQ.1)IPF=1
1346      GO TO 3413
1347  C WRITE SUMMARY FILE
1348  3600  CONTINUE
1349      UNIT=UNIT9
1350  C WRITE HEADERS
1351      WRITE(UNIT,3605)
1352  3605  FORMAT(' '//39X,'*** CMB SOURCE CONTRIBUTION SUMMARY ***'/' ')
1353  3613  WRITE(UNIT,3615)CMBID
1354  3615  FORMAT(' ',/,36X,'RESULTS FOR CMB SITE: ',3A4,5X,
1355      * 'YEAR: ',A2,3X,'DATE: ',A4)
1356  3617  FORMAT(1X,' ')
1357      WRITE(UNIT,3630)UDUR,USTART
1358  3630  FORMAT(
1359      *1X,30X,'SAMPLING DURATION: ',I2,' HRS. WITH START HOUR: ',I2)
1360      WRITE(UNIT,3640)YBACK(IBACK)
1361  3640  FORMAT(30X,'BACKGROUND SITE SUBTRACTED: ',A3)
1362      IF(IBACK.EQ.2)GO TO 3652
1363  C WRITE BACKG INFO
1364      WRITE(UNIT,3650)BACKID
1365  3650  FORMAT(30X,'BACKGROUND CMB SITE: ',3A4,5X,'YEAR: ',A2,3X,
1366      * 'DATE: ',A4)
1367      WRITE(UNIT,3630)BDUR,BSTART
1368  3652  CONTINUE
1369      IS1=IFLAG(1)+1
1370      IS2=IFLAG(2)+1
1371      WRITE(UNIT,3654)ISTAR(IS1),ISTAR(IS2)
1372  3654  FORMAT(/,1X,' SOURCE ',18X,'FINE',A4,26X,'COARSE',A4,25X,'TOTAL'/
1373      *1X,117(' ')/3(16X,'UG/M3',15X,'%'))
1374  C CALCULATE PERCENTS AND WRITE CONTRIBUTIONS
1375      FX=SAINT(1)
1376      CX=SAINT(2)
1377      TX=SAINT(3)
1378      WRITE(UNIT,3657)SAINT(1),USAINT(1),SAINT(2),USAINT(2),SAINT(3),
1379      * USAINT(3)
1380  3657  FORMAT(' INTERCEPT',3(1X,F7.3,' +- ',F7.3,18X))
1381      DO 3660 I=1,ISCTR
1382      J=ISHOLD(I)
1383      CALL PERC(FPCNT,UFPNT,USORC(J,1),UUSORC(J,1),UFMSS,UUFMSS)
1384      CALL PERC(CPCNT,UCPCNT,USORC(J,2),UUSORC(J,2),UCMSS,UUCMSS)
1385      CALL PERC(TPCNT,UTPCNT,USORC(J,3),UUSORC(J,3),UTMSS,UUTMSS)
1386      WRITE(UNIT,3658)SOUNAM(J),USORC(J,1),UUSORC(J,1),FPCNT,UFPNT,
1387      *USORC(J,2),UUSORC(J,2),CPCNT,UCPCNT,USORC(J,3),UUSORC(J,3),TPCNT,
1388      *UTPCNT
1389  3658  FORMAT(1X,A8,1X,6(1X,F7.3,' +- ',F7.3))
1390  C WRITE FILE FOR PCOMP COMMAND TO READ
1391      WRITE(UNIT10,3659)CMBID,J,SOUNAM(J),USORC(J,1),UUSORC(J,1),
1392      * USORC(J,2),UUSORC(J,2),USORC(J,3),UUSORC(J,3)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1393 3659 FORMAT(3A4,A2,A4,1X,I2,1X,A8,2X,6F8.3)
1394 C INCREMENT SUMS
1395     FX=FX+USORC(J,1)
1396     CX=CX+USORC(J,2)
1397     TX=TX+USORC(J,3)
1398 3660 CONTINUE
1399 C CALCULATE AND WRITE SUMS
1400     CALL PERC(FPCNT,UFCNT,FX,SET(1),UFMSS,UUFMSS)
1401     CALL PERC(CPCNT,UCPCNT,CX,SET(2),UCMSS,UUCMSS)
1402     CALL PERC(TPCNT,UTPCNT,TX,SET(3),UTMSS,UUTMSS)
1403     WRITE(UNIT,3664)FX,SET(1),FPCNT,UFCNT,CX,SET(2),CPCNT,UCPCNT,
1404     *TX,SET(3),TPCNT,UPCNT,UFMSS,UUFMSS,UCMSS,UUCMSS,UTMSS,UUTMSS
1405 3664 FORMAT(1X,117('-'))/,1X,'CALC.MASS',6(1X,F7.3,'+-',F7.3)/
1406     *1X,'MEAS.MASS',1X,3(F7.3,'+-',F7.3,19X)///)
1407     IF(IFLAG(1).EQ.1.OR.IFLAG(2).EQ.1)WRITE(UNIT,3671)(FLAG(I,2),I=1,8
1408     *)
1409     IF(IFLAG(1).EQ.2.OR.IFLAG(2).EQ.2)WRITE(UNIT,3672)(FLAG(I,3),I=1,8
1410     *)
1411 3671 FORMAT(//,' *NOTE: ',8A4)
1412 3672 FORMAT(//,' **NOTE: ',8A4)
1413 C WRITE MAGSTO FILE
1414 C CALCULATE INDIVIDUAL ELEMENTAL CONTRIBUTIONS FOR EACH SOURCE
1415 3676 DO 3680 I=1,ISCTR
1416     J=ISHOLD(I)
1417 C WRITE MASS CONTRIBUTION
1418     IX=01
1419     DO 3680 IEL=1,NEL
1420     DO 3677 ISIZ=1,2
1421     IF(A(IEI,J,ISIZ).LE.0.0E-09)SEL(ISIZ)=0.0
1422     IF(A(IEI,J,ISIZ).LE.0.0E-09)USEL(ISIZ)=0.0
1423     IF(A(IEI,J,ISIZ).LE.0.0E-09)GO TO 3677
1424     SEL(ISIZ)=A(IEI,J,ISIZ)*USORC(J,ISIZ)
1425     USEL(ISIZ)=SQRT(SEL(ISIZ)**2*((UA(IEI,J,ISIZ)/A(IEI,J,ISIZ))
1426     ***2+(UUSORC(J,ISIZ)/USORC(J,ISIZ))**2)
1427     * + (UA(IEI,J,ISIZ)*UUSORC(J,ISIZ))**2)
1428 3677 CONTINUE
1429     IF(SEL(1).EQ.0.0.AND.SEL(2).EQ.0.0)GO TO 3680
1430     WRITE(UNIT12,3678)CMBID,UDUR,USTART,SCODE(J),PCODE(IEI)
1431     *,SEL(1),USEL(1),SEL(2),USEL(2)
1432 3678 FORMAT('40',1X,3A4,1X,A2,A4,1X,I2,1X,I2,1X,I2,1X,
1433     *I2,2X,F9.4,2X,F9.4,2X,F9.4,2X,F9.4)
1434 3680 CONTINUE
1435 3995 GO TO(500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1436 C
1437 C
1438 C
1439 C
1440 C

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1441 C
1442 C
1443 C
1444 C      PART OF COMMAND PMATRIX
1445 C      PRINTS CURRENT FINE AND COARSE MEASURED CONCENTRATIONS
1446 3700 WRITE(UNITX,3710)CMBID
1447 3710 FORMAT(1H , 'CURRENT MEASURED UG/M3 CONCENTRATIONS FOR'/' SITE:',
1448 * 3A4,5X, 'YEAR: ',A2,2X, 'DATE: ',A4,
1449 */1X,71('-'),/,1H , 'SPECIES',14X, 'FINE',13X, 'COARSE',13X, 'TOTAL',
1450 */1X,71('-')//)
1451      DO 3730 I=1,NEL
1452      WRITE(UNITX,3720)I,ELMENT(I),UCNC(I,1),UUCNC(I,1),UCNC(I,2),
1453 *UUCNC(I,2),UCNC(I,3),UUCNC(I,3)
1454 3720      FORMAT(1H ,I2,1X,A8,1X,F8.3,'+-',F8.3,2(1X,F8.3,'+-',F8.3))
1455 3730      CONTINUE
1456      GO TO 43005
1457 C
1458 C
1459 C
1460 C
1461 C
1462 C      -CALCON.  CALCULATE CONCENTRATIONS.
1463 3800      DO 3850 IEL=1,NEL
1464      CLCN(IEI,SIZ)=SAINT(SIZ)
1465      UCLCN(IEI,SIZ)=0.0
1466      KSOURC=NSOURC
1467      DO 3840 JSOURC=1,KSOURC
1468      IF(UUSORC(JSOURC,SIZ).LE.0.)GO TO 3840
1469      CLCN(IEI,SIZ)=CLCN(IEI,SIZ)+A(IEI,JSOURC,SIZ)*USORC(JSOURC,SIZ)
1470      UCLCN(IEI,SIZ)=(UCLCN(IEI,SIZ)**2+(UA(IEI,JSOURC,SIZ)*USORC
1471 1(JSOURC,SIZ))**2)**.5
1472 3840      CONTINUE
1473 3850      CONTINUE
1474      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1475 C
1476 C
1477 C
1478 C
1479 C      -RESUM. GO BACK INTO AUTOFIT
1480 4000      ICNTRL=KCNTRL
1481      GO TO 4132
1482 C
1483 C
1484 C
1485 C
1486 C      -AUTOFIT.  STEPS THROUGH COMMAND SEQUENCE FOR A GIVEN SAMPLE
1487 4099      NOSKIP=0
1488 4100      CONTINUE

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1489 C IF END OF AUTOFIT DATA, WRITE TO SCREEN AND GO TO COMMAND
1490     IF(ICNTRL.NE.0)GO TO 4106
1491     WRITE(UNIT6,4105)
1492 4105 FORMAT(1H , 'AUTOFIT SEQUENCING FINISHED')
1493     ICNTRL=4
1494     IRTN=1
1495     GO TO 500
1496 4106 CONTINUE
1497 C IF FIRST SAMPLE GO TO SELECT
1498     IRTN=3
1499     IF(ICNTRL.NE.2)GO TO 4210
1500 C RETRIEVE NEXT CMBID FROM PREVIOUS DATA SEARCH
1501     DO 4110 I=1,5
1502 4110 CMBID(I)=SAVE(I)
1503 C CALL UP DATA
1504 4120 ICNTRL=1
1505     WRITE(UNIT6,4122)CMBID
1506 4122 FORMAT(1H , 'DATA SEARCH BEGUN FOR',/6X,'SITE: ',3A4,5X,
1507 * 'YEAR: ',A2,2X,'DATE: ',A4/)
1508     CALL FETCH(QUOTA,CMBID,UDUR,USTART,UCNC,
1509 *UUCNC,UFMSS,UUFMSS,UCMSS,UUCMSS,UTMSS,UUTMSS,MFLAG,
1510 *SAVE,ICNTRL,TYPE,UNIT6,UNIT12,UNIT13)
1511     IF(ICNTRL.EQ.9)IRTN=1
1512     IF(ICNTRL.EQ.9)GO TO 500
1513 4123 SIZ=1
1514 4124 CONTINUE
1515 C PERFORM CEB
1516 4130 IRTN=5
1517     GO TO 2801
1518 4132 NOSKIP=1
1519 C RETURN FROM RESUM- WRITE DATA, GO TO NEXT SIZE
1520 4135 IRTN=6
1521     GO TO 3400
1522 4150 CONTINUE
1523 CHECK IF DONE BOTH SIZES & RECYCLE AUTOFIT
1524     IF(SIZ.EQ.2)GO TO 4100
1525     SIZ=2
1526     GO TO 4124
1527 C
1528 C
1529 C
1530 C     -SELECT.  ALLOWS DATA SET SELECTION
1531 C
1532 4200 CONTINUE
1533     IRTN=7
1534 4210 WRITE(UNIT6,4215)
1535 4215 FORMAT(' ENTER DESIRED CMB SITE CODE: XXXXXXXXXXXXX')
1536     READ(UNIT5,4218,ERR=4210)SITE

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1537      WRITE(UNIT6,4216)
1538      READ(UNIT5,4217) YEAR
1539      WRITE(UNIT6,4219)
1540      READ(UNIT5,4220) DATE
1541      4216 FORMAT(' ENTER YEAR: YY')
1542      4217 FORMAT(A2)
1543      4219 FORMAT(' ENTER DATE: MMDD')
1544      4220 FORMAT(A4)
1545      4218 FORMAT(3A4)
1546      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1547      4250 IRTN=8
1548      C
1549      4254 WRITE(UNIT6,4255)
1550      4255 FORMAT(' INPUT DESIRED SIZE FRACTION:(FINE OR COARSE)')
1551      READ(UNIT5,28001,ERR=4254)ANS
1552      SIZ=1
1553      IF(ANS.EQ.2UOTC) SIZ=2
1554      ICNTRL=4
1555      WRITE(UNIT6,4122)CMBID
1556      CALL FETCH(2UOTS,CMBID,UDUR,USTART,UCNC,
1557      *UUCNC,UFMSS,UUFMSS,UCMSS,UUCMSS,UTMSS,UUTMSS,MFLAG,
1558      *DUM,ICNTRL,TYPE,UNIT6,UNIT12,UNIT13)
1559      IBACK=2
1560      IF (ICNTRL.EQ.9)IRTN=1
1561      IF(ICNTRL.EQ.9)GO TO 500
1562      C DO CMB
1563      4260 IRTN=9
1564      GO TO 2800
1565      4270 CONTINUE
1566      4280 CONTINUE
1567      C
1568      C
1569      C
1570      C
1571      C      -INITIAL. INITIALIZE FITTING SOURCES AND ELEMENTS
1572      4400 WRITE(UNIT6,3110)SIZNAM(SIZ)
1573      4401 DO 4410 IEL=1,NEL
1574      ELFT(IEI,SIZ)=IBLANK
1575      4410 ELHOLD(IEI,SIZ)=0
1576      DO 4420 JSOURC=1,NSOURC
1577      SOUFT(JSOURC,SIZ)=IBLANK
1578      4420 SOHOLD(JSOURC,SIZ)=0
1579      4430 MEL=IMEL
1580      MEL1(SIZ)=IMEL
1581      MSOURC=IMSO
1582      MSORC1(SIZ)=IMSO
1583      4440 DO 4450 KEL=1,MEL
1584      IEL=INITEL(KEL)

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1585      ELFT(IEL,SIZ)=STAR
1586      ELHOLD(KEL,SIZ)=IEL
1587  4450  CONTINUE
1588      DO 4460 KSOURC=1,MSOURC
1589      JSOURC=INITSO(KSOURC)
1590      SOUFT(JSOURC,SIZ)=STAR
1591      SOHOLD(KSOURC,SIZ)=JSOURC
1592  4460  CONTINUE
1593      IF(IRTN.EQ.0)GO TO 444
1594      GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1595  C
1596  C
1597  C
1598  C
1599  C
1600  C      -BACKOUT. SELECTS AND SUBTRACTS BACKGROUND
1601  4600  CONTINUE
1602      IF(IBACK.NE.2)GO TO 4670
1603  4602  WRITE(UNIT6,4605)
1604  4605  FORMAT(' ENTER BACKGROUND CMB SITE CODE: XXXXXXXXXXXXX')
1605      READ(UNIT5,4607,ERR=4602)BSITE
1606  4607  FORMAT(3A4)
1607      WRITE(UNIT6,4216)
1608      READ(UNIT5,4217) BYEAR
1609      WRITE(UNIT6,4219)
1610      READ(UNIT5,4220) BDATE
1611      ICNTRL=7
1612  4610  CALL FETCH(QUOTB,BACKID,BDUR,BSTART,BCNC,
1613      *UBCNC,BFMSS,UBFMSS,BCMSS,UBCMSS,BTMSS,UBTMSS,MFLAGB,
1614      *DUM,ICNTRL,TYPE,UNIT6,UNIT12,UNIT13)
1615      IF(ICNTRL.EQ.9)IRTN=1
1616      IF(ICNTRL.EQ.9)GO TO 500
1617      DO 4650 I=1,3
1618      DO 4650 IEL=1,NEL
1619      UCNC(IEL,I)=UCNC(IEL,I)-BCNC(IEL,I)
1620      UUCNC(IEL,I)=((UUCNC(IEL,I)**2)+UBCNC(IEL,I)**2)**.5
1621  4650  CONTINUE
1622      UFMSS=UFMSS-BFMSS
1623      UUFMSS=(UUFMSS**2+UBFMSS**2)**.5
1624      UCMSS=UCMSS-BCMSS
1625      UUCMSS=(UUCMSS**2+UBCMSS**2)**.5
1626      UTMSS=UTMSS-BTMSS
1627      UUTMSS=(UUTMSS**2+UBTMSS**2)**.5
1628      WRITE(UNIT6,4655)
1629  4655  FORMAT(' BACKOUT COMPLETE')
1630      GO TO 4680
1631  4670  WRITE(UNIT6,4675)
1632  4675  FORMAT(' CURRENT DATA ALREADY HAS BACKGROUND SUBTRACTED')

```

TABLE A.1 CMB MAIN PROGRAM

(CONTINUED)

```

1633 4680 IBACK=1
1634 GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1635 C
1636 C
1637 C
1638 C -BACKIN. ELIMINATES CURRENT BACKGROUND SUBTRACTION
1639 4700 CONTINUE
1640 IF(IBACK.NE.1)GO TO 4770
1641 DO 4750 I=1,3
1642 DO 4750 IEL=1,NEL
1643 UCNC(IEL,I)=UCNC(IEL,I)+BCNC(IEL,I)
1644 UUCNC(IEL,I)=((UUCNC(IEL,I)**2)-UBCNC(IEL,I)**2)**.5
1645 4750 CONTINUE
1646 UFMSS=UFMSS+BFMSS
1647 UUFMSS=(UUFMSS**2-UBFMSS**2)**.5
1648 UCMSS=UCMSS+BCMSS
1649 UUCMSS=(UUCMSS**2-UBCMSS**2)**.5
1650 UTMSS=UTMSS+BTMSS
1651 UUTMSS=(UUTMSS**2-UBTMSS**2)**.5
1652 WRITE(UNIT6,4755)
1653 4755 FORMAT(' BACKIN COMPLETE')
1654 GO TO 4780
1655 4770 WRITE(UNIT6,4775)
1656 4775 FORMAT(1H,'CURRENT CMB DATA DOES NOT HAVE BACKGROUND SUBTRACTED')
1657 4780 IBACK=2
1658 GO TO (500,2860,4120,4130,4132,4150,4250,4260,4270,4280),IRTN
1659 C
1660 C
1661 C
1662 C
1663 C - PCOMP
1664 C
1665 C
1666 COMPUTE MEAN AND STANDARD DEVIATION OF SERIES
1667 52000 UNIT=UNIT11
1668 WRITE(UNIT6,52001)
1669 52001 FORMAT(' OUTPUT WILL GO TO HARDCOPY.'/
1670 * ' DO YOU WANT IT DISPLAYED AT YOUR TERMINAL INSTEAD?')
1671 READ(UNIT5,28001)ANS
1672 IF(ANS.EQ.YESY)UNIT=UNIT6
1673 REWIND UNIT10
1674 DO 52005 I=1,MELMAX
1675 DO 52005 J=1,MSOMAX
1676 F(I,J)=0.0
1677 XP(I,J)=0.0
1678 52005 SF(I,J)=0.0
1679 K=0
1680 M=0

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1681 52010 READ(UNIT10,52011,END=53000)TEMPID,J,FINE,COARSE,TOTAL
1682 52011 FORMAT(3A4,3A2,1X,I2,11X,F8.3,8X,F8.3,8X,F8.3)
1683      DO 52020 I=1,6
1684      IF(TEMPID(I).NE.LASTID(I) .OR. K.EQ.0)GO TO 52030
1685 52020 CONTINUE
1686      GO TO 52040
1687 52030 K=K+1
1688      IF(K.GT.16)GO TO 53000
1689      DO 52032 I=1,6
1690      LASTID(I)=TEMPID(I)
1691      PNAM(K,I)=TEMPID(I)
1692 52032 CONTINUE
1693 52040 IF(M.GT.0)GO TO 52050
1694      ITM(1)=J
1695      M=1
1696      IEL=1
1697      GO TO 52060
1698 52050 DO 52052 I=1,M
1699      IF(J.EQ.ITM(I)) GO TO 52055
1700 52052 CONTINUE
1701      IF(M.GE.21)GO TO 52010
1702      M=M+1
1703      ITM(M)=J
1704      IEL=M
1705      GO TO 52060
1706 52055 IEL=I
1707 52060 F(IEL,K)=FINE
1708      XP(IEL,K)=COARSE
1709      SF(IEL,K)=TOTAL
1710      GO TO 52010
1711 53000 DO 53090 I=1,M
1712      WRITE(UNIT,53970)
1713 53970 FORMAT(/40X,'FINE',9X,'COARSE',7X,'TOTAL',/' ',3X,
1714      * 'CMB SITE',7X,'DATE',4X,'SOURCE',6X,'(UG/M3)',6X,
1715      * '(UG/M3)',6X,'(UG/M3)')
1716      X=0
1717      UX=0
1718      TX=0
1719      UTX=0
1720      PCNT=0
1721      UPCNT=0
1722      WRITE(UNIT,53972)
1723 53972 FORMAT(4X,8(' '),7X,4(' '),4X,6(' '),6X,7(' '),6X,7(' '),
1724      * 6X,7(' ')/)
1725      INDX=ITM(I)
1726      TEMPN=SOUNAM(INDX)
1727      DO 53080 J=1,K
1728      WRITE(UNIT,53978) (PNAM(J,IEL),IEL=1,6),TEMPN,F(I,J),XP(I,J),

```

TABLE A.1 CMB MAIN PROGRAM (CONTINUED)

```

1729      * SF(I,J)
1730 53978 FORMAT(2X,3A4,3X,A2,'/',A2,'/',A2,2X,A8,
1731      * 2X,F7.2,7X,F7.2,6X,F7.2)
1732      X=X+F(I,J)
1733      TX=TX+XP(I,J)
1734      PCNT=PCNT+SF(I,J)
1735      IF(K.LE.1)GO TO 53080
1736      UX=UX+F(I,J)**2
1737      UTX=UTX+XP(I,J)**2
1738      UPCNT=UPCNT+SF(I,J)**2
1739 53080 CONTINUE
1740      WRITE(UNIT,53988)
1741 53988 FORMAT(/39X,7('-'),6X,7('-'),6X,7('-'))
1742      IF(K.LE.1)GO TO 53989
1743      UX=SQRT((UX-X/K*X)/(K-1.))
1744      UTX=SQRT((UTX-TX/K*TX)/(K-1.))
1745      UPCNT=SQRT((UPCNT-PCNT/K*PCNT)/(K-1.))
1746      X=X/K
1747      TX=TX/K
1748      PCNT=PCNT/K
1749 53989 WRITE(UNIT,53990)X,TX,PCNT,UX,UTX,UPCNT
1750 53990 FORMAT(22X,'AVERAGE',8X,F7.2,7X,F7.2,6X,F7.2/20X,
1751      * '(STD. DEV.)',4X,'+-',F7.2,5X,'+-',F7.2,4X,'+-',F7.2/)
1752 53090 CONTINUE
1753      REWIND UNIT10
1754      IRTN=1
1755      GO TO 500
1756 C
1757 C
1758 5000 STOP
1759      END
1760 C
1761 C
1762 C

```

TABLE A.2 CMBR SUBROUTINE

```

1      SUBROUTINE CMBR(F,C,N,L,NN,LL,SF,V,VK,TOTALA,SSET,
2      * KSTARK,SAS,SAA,SR2,R2LS,VIF,
3      * RIDGE,EFVAR,INTCEP,IERR,KBUG,CWT,
4      * W,X,Y,XMEAN,XPX,XPXK,XPY,SX,S,TM,A,SOLD,IS,IA,ITM
5      * )
6      C      THIS SUBPROGRAM PERFORMS THE CMB ANALYSIS
7      C      OPTIONS ARE RIDGE REGRESSION,
8      C      EFFECTIVE VARIANCE METHOD,
9      C      AND INCLUSION OF INTERCEPT
10     C
11     C
12     C      WRITTEN BY D.A. DUBOSE AND H.J. WILLIAMSON
13     C      RADIAN CORPORATION,AUSTIN TEXAS IN 1982
14     C      UNDER CONTRACT TO EPA (PROJECT OFFICER W.P. FREAS)
15     C
16     C
17     C *****ARGUMENTS   TO THE SUBPROGRAM*****
18     C
19     C      ***** INPUT *****
20     C
21     C      F-SOURCE SIGNATURE MATRIX
22     C      C-CONCENTRATION VECTOR
23     C      SF-STANDARD ERROR OF F
24     C      V-STANDARD ERROR OF C
25     C      N-NUMBER OF SPECIES
26     C      L-NUMBER OF SOURCES
27     C      NN-MAXIMUM NUMBER OF SPECIES(ARRAY DIMENSION)
28     C      LL-MAXIMUM NUMBER OF SOURCES(ARRAY DIMENSION)
29     C      VK-VECTOR OF K-VALUES FOR RIDGE REGRESSION
30     C      TOTALA-TOTAL AEROSOL
31     C
32     C
33     C ***** CONTROL*****
34     C
35     C      RIDGE-RIDGE OPTION FLAG 0=NO 1=YES 2=YES +SUMMARY
36     C      EFVAR-EFFECTIVE VARIANCE FLAG 0=NO 1=YES
37     C      INTCEP-INTERCEPT OPTION FLAG 0=NO 1=YES
38     C      CWT-WEIGHT FOR RIDGE SOLUTION SELECTION
39     C      KBUG-NOT USED IN THIS VERSION
40     C
41     C
42     C ***** OUTPUT *****
43     C
44     C      SSET-STANDARD ERROR OF CALCULATED TOTAL AEROSOL
45     C      KSTARK-INDEX OF SELECTED RIDGE SOLUTION
46     C      SAS-MATRIX OF RIDGE SOLUTIONS
47     C      SAA-MATRIX OF STANDARD ERRORS OF SAS
48     C      SR2-R-SQUARE OF SELECTED RIDGE SOLUTION

```

TABLE A.2 CMBR SUBROUTINE

(CONTINUED)

```

49 C      R2LS-R-SQUARE OF LEAST SQUARES SOLUTION
50 C      VIF-VARIANCE INFLATION FACTORS
51 C      IERR-INVERSION ERROR FLAG
52 C
53 C
54 C ***** WORKSPACE *****
55 C
56 C      W-WEIGHTS
57 C      X-SCALED SIGNATURE
58 C      Y-SCALED CONCENTRATIONS
59 C      XMEAN-SOURCE MEANS
60 C      XPX-X'X MATRIX (CORRELATION MATRIX)
61 C      XPXK-XPX INVERSE
62 C      XPY-X'Y VECTOR
63 C      SX-SOURCE SCALE FACTORS
64 C      S-SOLUTION VECTOR
65 C      TM-MATRIX MULTIPLICATION WORK SPACE
66 C      A-STANDARD ERROR OF SOLUTION VECTOR S
67 C      SOLD -HOLDER FOR SOLUTION TO CHECK FOR CONVERGENCE
68 C      IA-WORKSPACE FOR INVERSION ROUTINE
69 C      ITM  -WORKSPACE FOR INVERSION ROUTINE
70 C      IS  -WORKSPACE FOR INVERSION ROUTINE
71 C
72 C
73 C
74 C ***** OTHER VARIABLES AND ARRAYS*****
75 C
76 C      ADIF-RIDGE SELECTION CLOSENESS CRITERIA VALUE
77 C      AINT-INTERCEPT
78 C      DET-ARGUMENT FOR INVERSION ROUTINE(DETERMINENT)
79 C      DF-DEGREES OF FREEDOM
80 C      EPS-ARGUMENT FOR INVERSION ROUTINE
81 C      IAGAIN-REITERATION FLAG
82 C      IBLANK-BLANK ' '
83 C      IN-NUMBER OF NEGATIVE SOLUTIONS
84 C      ITER-ITERATION NUMBER
85 C      KALL-NUMBER OF RIDGE K-VALUES
86 C      KINDEX - INDEX OF RIDGE SOLUTION
87 C      LP1-L PLUS ONE FOR INTERCEPT IF REQUESTED
88 C      MAXIT-MAXIMUM NUMBER OF ITERATIONS
89 C      MORE-NUMBER OF ADDITIONAL ITERATIONS
90 C      MSE-MEAN SQUARE ERROR
91 C      NPIV,PIV-ARGUMENTS FOR INVERSE ROUTINE
92 C      SE-STANDARS ERROR(SQRT MSE)
93 C      SET-STANDARD ERROR OF CALCULATED TOTAL AEROSOL
94 C      SSE-SUM OF SQUARES FOR ERROR
95 C      SY-CONCENTRATION SCALE FACTOR
96 C      SYSX-SCALE FACTOR FOR COEFFICIENTS

```

TABLE A.2 CMBR SUBROUTINE

(CONTINUED)

```

97 C      UNIT5,UNIT6-FORTRAN READ/WRITE UNITS
98 C      WORST-VALUE OF NEGATIVE COEFFICIENTS OF GREATEST MAGNITUDE
99 C      WT-WEIGHT(OFTEN USED AS WORK VARIABLE)
100 C      STARK-K-VALUE OF BEST RIDGE SOLUTION TO DATE
101 C      SUMNEG-NEGATIVE COEFFICIENT RIDGE SELECTION CRITERIA VALUE
102 C      SUMWT-RIDGE SELECTION CLOSENESS(ALSO WORK SPACE)
103 C      SXM-WORK VARIABLE
104 C
105 C *****
106       REAL F(NN,LL), C(NN), V(NN), SF(NN,LL), VK(31),
107       * X(NN,LL),SAS(LL,31),SAA(LL,31),VIF(LL),
108       * Y(NN),XMEAN(LL),XPX(LL,LL),XPXK(LL,LL),
109       * XPY(LL), SX(LL), S(LL), TM(NN), A(LL), SOLD(LL),W(NN),SSET(2)
110       INTEGER IS(LL),IA(LL),ITM(NN),UNIT5,UNIT6
111       REAL K,MSE
112       INTEGER EFVAR,RIDGE
113       DATA IBLANK/' '/
114 C
115       UNIT5=5
116       UNIT6=6
117       KALL=31
118 C
119       EPS=0.
120       ADIFF=1.E30
121       KINDEX=1
122       DO 2020 I=1,N
123         W(I)=V(I)
124       2020 CONTINUE
125       KBUG=0
126       CONTROL POINT - BEGIN CYCLE FOR K-VALUE
127       3000 CONTINUE
128         K=VK(KINDEX)
129         MAXIT=10
130         ITER=1
131         IF(EFVAR.EQ.0 .AND. KINDEX.GT.1) GO TO 9000
132       CONTROL POINT - BEGIN ITERATION LOOP
133       4000 CONTINUE
134       COMPUTE WEIGHTS & WEIGHTED MEANS
135         SUMWT=0.
136         YMEAN=0.
137         DO 5005 J=1,L
138       5005 XMEAN(J)=0.
139         DO 5008 I=1,N
140         W(I)=1./W(I)
141       5008 CONTINUE
142         LP1=L
143         IF(INTCEP.EQ.0) GO TO 6000
144       CORRECT SOURCE MATRIX TO INCLUDE INTERCEPT TERM

```

TABLE A.2 CMBR SUBROUTINE

(CONTINUED)

```
145      LP1=L+1
146      DO 5020 I=1,N
147      F(I,LP1)=1.0
148      5020 CONTINUE
149      6000 CONTINUE
150  CALCULATE VARIANCE STABILIZATION BY WEIGHTING
151      DO 6020 I=1,N
152      DO 6010 J=1,LP1
153      X(I,J) = F(I,J)*W(I)
154      6010 CONTINUE
155      Y(I)=C(I)*W(I)
156      6020 CONTINUE
157  COMPUTE STANDARDIZING FACTORS
158      DO 6060 J=1,LP1
159      WT=0.
160      DO 6050 I=1,N
161      WT=WT+X(I,J)**2
162      6050 CONTINUE
163      SX(J)=SQRT(WT)
164      6060 CONTINUE
165      SY=0.
166      DO 6070 I=1,N
167      SY=SY+Y(I)**2
168      6070 CONTINUE
169      SY=SQRT(SY)
170  COMPUTE STANDARDIZED DATA VALUES
171      DO 6090 I=1,N
172      DO 6080 J=1,LP1
173      X(I,J)=X(I,J)/SX(J)
174      6080 CONTINUE
175      Y(I)=Y(I)/SY
176      6090 CONTINUE
177  COMPUTE MATRIX OF SUM OF SQUARES AND CROSS PRODUCTS
178      DO 7030 J=1,LP1
179      DO 7020 M=1,J
180      WT=0
181      DO 7010 I=1,N
182      WT=WT + X(I,M) * X(I,J)
183      7010 CONTINUE
184      XPX(M,J) = WT
185      XPX(J,M) = WT
186      7020 CONTINUE
187      WT=0
188      DO 7025 I=1,N
189      WT=WT + X(I,J)*Y(I)
190      7025 CONTINUE
191      XPY(J)=WT
192      7030 CONTINUE
```

```

193 CHECKPOINT - ADD RIDGE TO SSCP MATRIX
194   9000 CONTINUE
195     DO 9050 M=1,LP1
196       I=M-1
197       DO 9040 J=1,I
198         XPXK(M,J)=XPX(M,J)
199         XPXK(J,M)=XPX(M,J)
200   9040 CONTINUE
201     XPX(M,M)=1.0 + K
202     XPXK(M,M)=XPX(M,M)
203   9050 CONTINUE
204 CALL INVERSE ROUTINE
205     CALL INV1(XPXK,LP1,LL,EPS,IS,IERR,DET,NPIV,PIV,IA,ITM)
206     IF(IERR.EQ.0)GO TO 10000
207     WRITE(UNIT6,9090)
208   9090 FORMAT(' ***ERROR: SINGULAR MATRIX, CHECK DATA')
209     IERR=1
210     GO TO 99900
211 COMPUTE SOLUTION VECTOR
212   10000 CONTINUE
213     DO 10020 J=1,LP1
214       WT=0.
215       DO 10010 M=1,LP1
216         WT=WT + XPXK(J,M)*XPY(M)
217   10010 CONTINUE
218     S(J)=WT
219   10020 CONTINUE
220 COMPUTE R-SQUARED
221     SSE=0.
222     DO 12020 I=1,N
223       WT=0.
224       DO 12010 J=1,LP1
225         WT=WT + X(I,J)*S(J)
226   12010 CONTINUE
227       WT=Y(I)-WT
228       SSE=SSE+WT*WT
229   12020 CONTINUE
230     WT=0.
231     IF(INTCEP.EQ.1)WT=XPY(LP1)**2
232     R2=1-SSE/(1-WT)
233     DF=N-LP1
234     MSE=SSE/DF
235     SE=SQRT(MSE)
236 COMPUTE STANDARD ERRORS
237     SET=0.0
238     DO 14030 M=1,LP1
239       DO 14020 J=1,LP1
240         WT=0

```

```

241      DO 14010 I=1,LP1
242      WT=WT + XPXK(M,I)*XPX(I,J)
243 14010 CONTINUE
244      TM(J)=WT - K*XPXK(M,J)
245 14020 CONTINUE
246      WT=0
247      DO 14025 J=1,LP1
248      WT= WT + TM(J)*XPXK(J,M)
249 COMPUTE DATA SCALE STANDARD ERROR OF TOTAL AEROSOL
250      SXM=SX(M)
251      DO 14025 I=1,LP1
252      SET=SET+TM(J)/SXM*XPXK(J,I)/SX(I)
253 14025 CONTINUE
254      A(M)=SE*SQRT(WT)
255 14030 CONTINUE
256      SET=SQRT(SY*SET)
257 COMPUTE DATA SCALE SOLUTION AND STANDARD ERRORS
258      AINT=0.0
259      DO 16020 J=1,LP1
260      SYSX=SY/SX(J)
261      S(J)=S(J)*SYSX
262      A(J)=A(J)*SYSX
263 16020 CONTINUE
264      IF(INTCEP.NE.0)AINT=S(LP1)
265 COMPUTE EFFECTIVE VARIANCES
266      IF(EFVAR.EQ.0) GO TO 20000
267      DO 17030 I=1,N
268      WT=V(I)**2
269      DO 17020 J=1,L
270      SYSX=S(J)*SF(I,J)
271      WT=WT + SYSX*SYSX
272 17020 CONTINUE
273      W(I)=SQRT(WT)
274 17030 CONTINUE
275 CHECK FOR CONVERGENCE
276      IAGAIN=0
277      IF(ITER.EQ.1) GO TO 18050
278      DO 18030 J=1,LP1
279      WT=ABS(S(J)-SOLD(J))/A(J)
280      IF(WT.GT. 0.1) IAGAIN=1
281 18030 CONTINUE
282      IF(IAGAIN.EQ.0 .OR. ITER.GE.MAXIT) GO TO 20000
283 18050 ITER=ITER+1
284      DO 18070 J=1,LP1
285      SOLD(J)=S(J)
286 18070 CONTINUE
287 CIRCLE BACK FOR ANOTHER ITERATION
288      GO TO 4000

```

```

289 COMPLETED ITERATION FOR THIS K
290 20000 CONTINUE
291     SSE=SSE*SY*SY
292 COMPUTE TOTAL AEROSOL AND # NEGATIVE COEFFICIENTS
293     WORST=0.
294     SUMNEG=0.
295     IN=0
296     SUMWT=0.
297     DO 20080 J=1,L
298     IF(S(J).GE.0.)GO TO 20078
299     IN=IN+1
300     SUMNEG=SUMNEG+S(J)*S(J)
301     IF(S(J).LT.WORST) WORST=S(J)
302 20078 SUMWT=SUMWT+S(J)
303 20080 CONTINUE
304     SUMWT=SUMWT+AIN
305     IF(RIDGE.NE.2) GO TO 21099
306     IF(KINDEX.EQ.1)WRITE(UNIT6,21085)
307 21085 FORMAT(/' RIDGE K',2X,'R-SQUARE',3X,'AEROSOL',3X,'SE(AEROSOL)',
308 * 2X,'# NEG',4X,'WORST',2X,'ITERATIONS')
309     WRITE(UNIT6,21086)K,R2,SUMWT,SET,IN,WORST,ITER
310 21086 FORMAT(2X,F5.3,4X,F6.4,3X,F8.3,3X,F8.2,6X,I2,F11.3,5X,
311 * I3)
312 21099 CONTINUE
313     IF(ITER.LT.MAXIT .OR. IAGAIN.EQ.0)GO TO 28000
314 22149 IF(RIDGE.GT.0)WRITE(UNIT6,22150)ITER,K
315 22150 FORMAT(' ',I3,' ITERATIONS SO FAR FOR RIDGE K=',F5.3,
316 * ' WITHOUT CONVERGENCE'/' HOW MANY MORE DO YOU WANT TO ',
317 * 'TRY?')
318     IF(RIDGE.EQ.0)WRITE(UNIT6,22151)ITER
319 22151 FORMAT(' ',I3,' ITERATIONS SO FAR WITHOUT CONVERGENCE'/'
320 * ' HOW MANY MORE DO YOU WANT TO TRY?')
321     READ(UNIT5,22152,ERR=22149)MORE,I
322 22152 FORMAT(I2,T2,A1)
323     IF(I.EQ.IBLANK)MORE=MORE/10
324     ITER=ITER+1
325     MAXIT=MAXIT+MORE
326     IF (MAXIT.GT.ITER)GO TO 4000
327 28000 CONTINUE
328 CHOCK AWAY COEFFICIENTS, ETC. FOR THIS RIDGE K SOLUTION
329     IF(KINDEX.EQ.1)SSET(1)=SET
330     DO 27030 J=1,LP1
331     SAS(J,KINDEX)=S(J)
332     SAA(J,KINDEX)=A(J)
333 27030 CONTINUE
334 COMPUTE VARIANCE INFLATION FACTORS
335     IF(K.NE.0.0) GO TO 27050
336     R2LS=R2

```

TABLE A.2 CMBR SUBROUTINE

(CONTINUED)

```
337      DO 27040 J=1,L
338      VIF(J)=XPXK(J,J)
339 27040 CONTINUE
340 27050 CONTINUE
341 CHOOSE BETTER SOLUTION
342      SUMWT=(SUMWT-TOTALA)**2 + CWT*SUMNEG
343      IF(SUMWT.GT.ADIFF) GO TO 40000
344      ADIFF=SUMWT
345      STARK=K
346      KSTARK=KINDEX
347      SR2=R2
348      SSET(2)=SET
349 CHECK FOR LAST OF K-SOLUTIONS
350 40000 CONTINUE
351      IF(KALL.LE.KINDEX .OR. RIDGE.EQ.0) GO TO 50000
352      KINDEX=KINDEX+1
353 CIRCLE BACK FOR ANOTHER K-VALUE
354      GO TO 3000
355 COMPLETED ALL K-VALUES
356 50000 CONTINUE
357      IF(RIDGE.GE.2)WRITE(UNIT6,50010) STARK
358 50010 FORMAT('ORIDGE K= ',F5.3,' IS THE SELECTED BEST SOLUTION')
359 99900 RETURN
360      END
```

TABLE A.3 FETCH SUBROUTINE

```

1  C
2  C
3  C
4  C  FETCH - ACCESSES INPUT DATA STORAGE
5  C
6  C  MODIFIED 1982 BY D.A. DUBOSE OF RADIAN CORP,AUSTIN TX
7  C  UNDER CONTRACT TO US EPA
8  C
9  C
10 C  ICNTRLS:
11 C      0- AUTOFIT EOF
12 C      1- AUTOFIT START
13 C      2- AUTOFIT IN MID SEARCH
14 C      4- SELECT START
15 C      5- SELECT IN MID SEARCH
16 C      7- BAGKGROUND START
17 C      8- BAGKGROUND IN MID SEARCH
18 C      9- DATA SEARCH FAILED
19 C
20 C      SUBROUTINE FETCH(ASB,INID,DUR,START,
21 C      *CONC,UCONC,FMASS,UFMASS,CMASS,UCMASS,TMASS,UTMASS,
22 C      *MFLAG,SAVE,ICNTRL,TYPE,UNIT6,UNIT12,UNIT13)
23 C
24 C
25 C      REAL*4 FMASS,UFMASS,CMASS,UCMASS,TMASS,UTMASS,CONC(35,3),
26 C      *UCONC(35,3),
27 C      *T10,T7,T8,T9
28 C
29 C
30 C
31 C
32 C  CHARACTER VARIABLES
33 C      INTEGER*4 ASB,SAVE(5),TYPE
34 C      * ,MFLAG(35,3),
35 C      * QUOTM,BLANK,QUOTB,QUOTA,QUOTS,QUOTFT,QUOTFC
36 C  INTEGER SPECS
37 C      INTEGER*4  T0,T6,SCODE(35),PCODE(35),DUR,START,
38 C      * UNIT6,UNIT12,UNIT13
39 C  CHARACTER VARIABLE SPECS
40 C      INTEGER*4 INID(5),ID(5)
41 C
42 C      COMMON /F/ PCODE,SCODE,NEL
43 C
44 C      EQUIVALENCE (SITE,INID(1)),(YEAR,INID(4)),(DATE,INID(5))
45 C
46 C  DATA INITIALIZATION
47 C      DATA QUOTM,BLANK,QUOTB,QUOTA,QUOTS,QUOTFT,QUOTFC /
48 C      *  'M',' ','B','A','S','FT','FC'/

```

TABLE A.3 FETCH SUBROUTINE (CONTINUED)

```

49  C
50  C
51  C
52  C
53  C
54  C    FORMAT STATEMENTS
55  C    TITLE CARD FOR SITE NUMBER AND YEAR AND DATE
56      25 FORMAT(5X,' SITE: ',3A4,5X,'YEAR: ',A2,2X,'DATE: ',A4,5X,A2)
57  C    POLLUTANT DATA CARDS
58      155    FORMAT(I2,1X,3A4,1X,A2,A4,1X,I2,1X,I2,4X,I2,2X,
59              *F9.4,2X,F9.4,2X,F9.4,2X,F9.4)
60  C
61  C
62  C    DATA SEARCH FAILURE
63      410    FORMAT(1H,'DATA SET NOT FOUND FOR'/6X,'SITE: ',
64              *    3A4,5X,'YEAR: ',A2,2X,'DATE: ',A4/
65              *    ' USE ONE OF THOSE LISTED ABOVE')
66  C
67  C
68  C
69  C
70  C
71  C    INITIALIZE CONCS,MASSSES AND MISSING DATA FLAGS
72      DO 3 I=1,NEL
73      DO 3 J=1,3
74      CONC(I,J)=0.000
75      UCONC(I,J)=0.001
76      MFLAG(I,J)=2QUOTM
77      3    CONTINUE
78      FMASS=0.000
79      UFMASS=0.000
80      CMASS=0.000
81      UCMASS=0.000
82      TMASS=0.000
83      UTMASS=0.000
84  C
85  C
86  C
87  C
88  C
89  C
90  C
91  C    REWIND DATA FILE
92      4    REWIND UNIT13
93  C
94  C
95  C
96  C

```

TABLE A.3 FETCH SUBROUTINE (CONTINUED)

```

97  C  READ DATA LINE
98  10  READ (UNIT13,155,END=200)T0,ID,IDUR,ISTART,T6,T7,T8,T9,T10
99  C
100 C
101 C
102 C
103 C
104 C
105 C
106 C
107 C
108 C  ROUTE CARD TYPES
109     IF(T0.EQ.3)GO TO 30
110     IF(T0.EQ.30.AND.ICNTRL.EQ.2)GO TO 150
111     IF(T0.EQ.30.AND.ICNTRL.EQ.5)GO TO 150
112     IF(T0.EQ.30.AND.ICNTRL.EQ.8)GO TO 150
113     GO TO 10
114 C
115 C
116 C
117 C
118 CONTROL POINT - CARD TYPE 3 (SITE HEADER CARD)
119     30 CONTINUE
120     DO 35 I=1,5
121     SAVE(I)=ID(I)
122     35 CONTINUE
123 C  CHECK CONTROLS
124     IF(ICNTRL.EQ.2)GO TO 320
125     IF(ICNTRL.EQ.8)GO TO 320
126     IF(ICNTRL.EQ.5)GO TO 320
127     TYPE=QUOTFC
128     IF(T6.EQ.13)TYPE=QUOTFT
129     WRITE(UNIT6,25)ID,TYPE
130 C MATCH INID
131     DO 37 I=1,5
132     IF(ID(I).NE.INID(I))GO TO 10
133 37 CONTINUE
134     DUR=IDUR
135     START=ISTART
136     IF(ASB.NE.QUOTB)WRITE(UNIT12,155) T0,ID,DUR,START,T6
137 C ADJUST CONTROLS
138     IF(ASB.EQ.QUOTA)ICNTRL=2
139     IF(ASB.EQ.QUOTB)ICNTRL=8
140     IF(ASB.EQ.QUOTS)ICNTRL=5
141 C  BACK TO READ
142     GO TO 10
143 C
144 C

```

TABLE A.3 FETCH SUBROUTINE (CONTINUED)

```

145  C
146  C
147  C
148  C
149  C
150  C
151  C   POLLUTANT CARDS
152  150   CONTINUE
153  C   CHECK IF POLLUTANT IS MASS
154      IF(T6.NE.01)GO TO 168
155  C
156  165   IF(TYPE .NE. 2)GO TO 167
157      FMASS=T7
158      UFMASS=T8
159      TMASS=T9
160      UTMASS=T10
161      CALL COARS(CMASS,UCMASS,TMASS,UTMASS,FMASS,UFMASS)
162      GO TO 168
163  167   FMASS=T7
164      UFMASS=T8
165      CMASS=T9
166      UCMASS=T10
167      TMASS=CMASS+FMASS
168      UTMASS=SQR(T(CMASS*UCMASS+UFMASS*UFMASS))
169      GO TO 168
170  C MATCH POLLUTANT CONCENTRATIONS
171  168   DO 172 I=1,NEL
172      IF(T6.E2.PCODE(I))GO TO 169
173      GO TO 172
174  169   IF(TYPE .NE. 2)GO TO 170
175      CONC(I,1)=T7
176      UCONC(I,1)=T8
177      CONC(I,3)=T9
178      UCONC(I,3)=T10
179      IF(CONC(I,1).E2.0.000.AND.UCONC(I,1).E2.0.000)UCONC(I,1)=000.001
180      IF(CONC(I,3).E2.0.000.AND.UCONC(I,3).E2.0.000)UCONC(I,3)=000.001
181      CALL COARS(CONC(I,2),UCONC(I,2),CONC(I,3),UCONC(I,3),
182      *CONC(I,1),UCONC(I,1))
183      GO TO 171
184  170   CONC(I,1)=T7
185      UCONC(I,1)=T8
186      CONC(I,2)=T9
187      UCONC(I,2)=T10
188      CONC(I,3)=CONC(I,1)+CONC(I,2)
189      UCONC(I,3)=SQR(T(UCONC(I,1)**2+UCONC(I,2)**2))
190      IF(CONC(I,1).E2.0.000.AND.UCONC(I,1).E2.0.000)UCONC(I,1)=000.001
191      IF(CONC(I,2).E2.0.000.AND.UCONC(I,2).E2.0.000)UCONC(I,2)=000.001
192      IF(CONC(I,3).E2.0.000.AND.UCONC(I,3).E2.0.000)UCONC(I,3)=000.001

```

TABLE A.3 FETCH SUBROUTINE

(CONTINUED)

```
193  C ADJUST MISSING DATA FLAGS
194  171    MFLAG(I,1)=BLANK
195        MFLAG(I,2)=BLANK
196        MFLAG(I,3)=BLANK
197  172    CONTINUE
198  C IF SELECT OR AUTOFIT,WRITE TEMP LINE
199  175    IF(ASB.NE.'B')WRITE(UNIT12,155)T0,INID,DUR,START,T6,T7,T8,T9,
200        * T10
201  C ADJUST CONTROLS
202        IF(ASB.EQ.'A')ICNTRL=2
203        IF(ASB.EQ.'B')ICNTRL=8
204        IF(ASB.EQ.'S')ICNTRL=5
205  C BACK TO READ
206        GO TO 10
207  C
208  C
209  C
210  C
211  C
212  C
213  C   END OF FILE
214  200    IF(ICNTRL.EQ.1)GO TO 400
215        IF(ICNTRL.EQ.7)GO TO 400
216        IF(ICNTRL.EQ.4)GO TO 400
217        IF(ICNTRL.EQ.2)ICNTRL=0
218        GO TO 320
219  C
220  C
221  C
222  C
223  C
224  C
225  C RETURN TO MAIN
226  320    RETURN
227  C
228  C
229  C   DATA SEARCH FAILED
230  400    WRITE(UNIT6,410)INID
231        ICNTRL=9
232        RETURN
233        END
234  C
```

TABLE A.4 COARS SUBROUTINE

```

1  C  SUBROUTINE COARS
2  C  FOR PROGRAM CMB
3  C  BY DR. J.G.WATSON
4  C    GETS COARSE FRACTION AND UNCERTAINTY
5  C
6      SUBROUTINE COARS(X,UX,TCONC,UTCONC,FCONC,UFCONC)
7      IF(UTCONC.EQ.-1..OR.UFCONC.EQ.-1.)GO TO 10
8      X=TCONC-FCONC
9      UX=(UTCONC**2+UFCONC**2)**.5
10     IF(X.LT.UX)X=UX/2.
11     RETURN
12 10   X=-1.
13     UX=-1.
14     RETURN
15     END

```

TABLE A.5 PERC SUBROUTINE

```

1  C
2  C
3  C
4  C SUBROUTINE PERC
5  C FOR PROGRAM CMB
6  C BY D. W. TORKELOSON
7  C   THIS ROUTINE CALCULATES PERCENTS AND THEIR UNCERTAINTIES
8  C
9      SUBROUTINE PERC(PCNT,UPCNT,X1,UX1,X2,UX2)
10     REAL*4 PCNT,UPCNT,X1,UX1,X2,UX2
11     IF(X2.EQ.0.)GO TO 5
12     IF(X1.EQ.-1..OR.X2.EQ.-1.)GO TO 15
13     PCNT=100.*(X1/X2)
14     UPCNT=100.*((UX1/X2)**2+(UX2*X1/X2**2)**2)**.5
15     IF(PCNT.LT.UPCNT)PCNT=UPCNT/2.
16     GO TO 10
17 5    PCNT=0.
18     UPCNT=0.
19 10   RETURN
20 15   PCNT=-1.
21     UPCNT=-1.
22     RETURN
23     END
24  C

```

TABLE A.6 INV1 SUBROUTINE

1	SUBROUTINE INV1(A,N,NN,EPS,LTEMP,IERR,DET,NPIV,PIV,LPR,LPC)	INVO
2	DIMENSION A(NN,NN)	INVO
3	DIMENSION LTEMP(1),LPR(1),LPC(1)	INVO
4	C	INVO
5	C DECK 8045A	INVO
6	C	INVO
7	C SUBROUTINES CALLED - NONE	INVO
8	C	INVO
9	C THIS ROUTINE INVERTS MATRIX A IN ITS OWN SPACE. IT ALSO COMPUTES THE	INVO
10	C THE DETERMINANT OF A.	INVO
11	C	INVO
12	C THE METHOD IS THE USUAL GAUSSIAN EXCHANGE PROCESS. BOTH ROWS AND	INVO
13	C COLUMNS ARE SEARCHED FOR MAXIMAL PIVOTS. THERE IS NO UNNECESSARY	INVO
14	C INTERCHANGING OF ROWS OR COLUMNS, ALL SUCH INTERCHANGES BEING CARRIED	INVO
15	C OUT AFTER THE EXCHANGE PROCESS IS COMPLETE. CHAPTER 1 OF E.L. STIEFLE,	INVO
16	C INTRODUCTION TO NUMERICAL MATHEMATICS, ACADEMIC PRESS, N.Y., 1963, SHOULD	INVO
17	C BE HELPFUL IN FOLLOWING THE CODE.	INVO
18	C	INVO
19	C THE CALLING PROGRAM MUST SET A,N,NN,EPS, AND LTEMP TO--	INVO
20	C	INVO
21	C A-THE MATRIX TO BE INVERTED	INVO
22	C	INVO
23	C N-THE ORDER OF A	INVO
24	C	INVO
25	C NN-THE NUMBER OF WORDS OF STORAGE PROVIDED FOR EACH COLUMN	INVO
26	C OF ARRAY A BY THE CALLING PROGRAM	INVO
27	C	INVO
28	C EPS-A NON-NEGATIVE NUMBER WHICH EACH PIVOT IS REQUIRED TO EXCEED	INVO
29	C IN ABSOLUTE VALUE (CUSTOMARILY ZERO)	INVO
30	C	INVO
31	C LTEMP-A BLOCK OF AT LEAST N WORDS OF TEMPORARY INTEGER STORAGE	INVO
32	C	INVO
33	C IN ADDITION TO OVERWRITING A WITH ITS INVERSE, THE ROUTINE ALSO SETS	INVO
34	C IERR, DET, NPIV, PIV, LPR, AND LPC TO--	INVO
35	C	INVO
36	C IERR- 0 IF INVERSION IS COMPLETED AND NO TROUBLE IS DETECTED	INVO
37	C	INVO
38	C 2 IF MAGNITUDE OF CURRENT PIVOT FAILS TO EXCEED EPS	INVO
39	C (INVERSION WILL NOT BE COMPLETED)	INVO
40	C	INVO
41	C DET-PLUS OR MINUS THE PRODUCT OF THE CURRENT AND ALL PREVIOUS	INVO
42	C PIVOTS	INVO
43	C	INVO
44	C NPIV-THE NUMBER OF THE CURRENT PIVOT (FIRST, SECOND, ETC.)	INVO
45	C	INVO
46	C PIV-THE CURRENT PIVOT	INVO
47	C	INVO
48	C LPR-THE FIRST NPIV POSITIONS LIST THE PIVOT ROW INDICES IN ORDER	INVO

TABLE A.6 INV1 SUBROUTINE

(CONTINUED)

49	C	OF USE	INV01
50	C		INV01
51	C	LPC-THE FIRST NPIV POSITIONS LIST THE PIVOT COLUMN INDICES IN	INV01
52	C	ORDER OF USE	INV01
53	C		INV01
54	C	DO INITIALIZATIONS	INV01
55	C		INV01
56		IERR=0	INV01
57		DET=1.	INV01
58		DO 2 I=1,N	INV01
59		LPR(I)=I	INV01
60		2 LPC(I)=I	INV01
61	C		INV01
62	C	BEGIN EXCHANGE PROCESS	INV01
63	C		INV01
64		DO 17 NP=1,N	INV01
65		NPIV=NP	INV01
66	C		INV01
67	C	SELECT PIVOT	INV01
68	C		INV01
69		PIV=0.	INV01
70		DO 4 K=NP,N	INV01
71		I=LPR(K)	INV01
72		DO 4 L=NP,N	INV01
73		J=LPC(L)	INV01
74		IF (ABS(A(I,J))-ABS(PIV)) 4,3,3	INV01
75		3 KPIV=K	INV01
76		LPIV=L	INV01
77		IPIV=I	INV01
78		JPIV=J	INV01
79		PIV=A(I,J)	INV01
80		4 CONTINUE	INV01
81	C		INV01
82	C	UPDATE DETERMINANT AND PIVOT ROW AND COLUMN LISTS	INV01
83	C		INV01
84		DET=DET*PIV	INV01
85		ITEMP=LPR(NP)	INV01
86		LPR(NP)=LPR(KPIV)	INV01
87		LPR(KPIV)=ITEMP	INV01
88		ITEMP=LPC(NP)	INV01
89		LPC(NP)=LPC(LPIV)	INV01
90		LPC(LPIV)=ITEMP	INV01
91	C		INV01
92	C		INV01
93	C	EXIT IF PIVOT TOO SMALL	INV01
94	C		INV01
95		IF (EPS-ABS(PIV)) 8,7,7	INV01
96		7 IERR=2	INV01

(CONTINUED)

```

97      RETURN
98      C
99      C MODIFY PIVOT ROW
100     C
101         8 DO 9 J=1,N
102         9 A(IPIV,J)=-A(IPIV,J)/PIV
103     C
104     C MODIFY OTHER ROWS
105     C
106         DO 14 I=1,N
107         IF(I-IPIV)10,14,10
108         10 TEMP=A(I,JPIV)
109         IF(TEMP)11,14,11
110         11 DO 13 J=1,N
111         IF(J-JPIV)12,13,12
112         12 A(I,J)=A(I,J)+A(IPIV,J)*TEMP
113         13 CONTINUE
114         14 CONTINUE
115     C
116     C MODIFY PIVOT COLUMN
117     C
118         DO 15 I=1,N
119         15 A(I,JPIV)=A(I,JPIV)/PIV
120         A(IPIV,JPIV)=-A(IPIV,JPIV)
121         17 CONTINUE
122     C
123     C END EXCHANGE PROCESS
124     C
125     C UNSCRAMBLE ROWS OF INVERSE AND ADJUST SIGN OF DETERMINANT
126     C
127         DO 18 I=1,N
128         L=LPR(I)
129         18 LTEMP(L)=LPC(I)
130         DO 22 I=1,N
131         19 K=LTEMP(I)
132         IF(I-K)20,22,20
133         20 DET=-DET
134         DO 21 J=1,N
135         TEMP=A(I,J)
136         A(I,J)=A(K,J)
137         21 A(K,J)=TEMP
138         LTEMP(I)=LTEMP(K)
139         LTEMP(K)=K
140         GO TO 19
141         22 CONTINUE
142     C
143     C UNSCRAMBLE COLUMNS OF INVERSE
144     C

```

[illegible]

TABLE A.6 INV1 SUBROUTINE (CONTINUED)

145	DO 23 I=1,N	INV10
146	L=LPC(I)	INV10
147	23 LTEMP(L)=LPR(I)	INV10
148	DO 27 I=1,N	INV10
149	24 K=LTEMP(I)	INV10
150	IF(I-K)25,27,25	INV10
151	25 DO 26 J=1,N	INV10
152	TEMP=A(J,I)	INV10
153	A(J,I)=A(J,K)	INV10
154	26 A(J,K)=TEMP	INV10
155	LTEMP(I)=LTEMP(K)	INV10
156	LTEMP(K)=K	INV10
157	GO TO 24	INV10
158	27 CONTINUE	INV10
159	RETURN	INV10
160	END	INV10

APPENDIX B

SELECTED FLOW DIAGRAMS

The diagrams presented in this appendix show the relationships among commands, input/output units and subprograms. The diagrams do not give specific details but overall concepts instead.

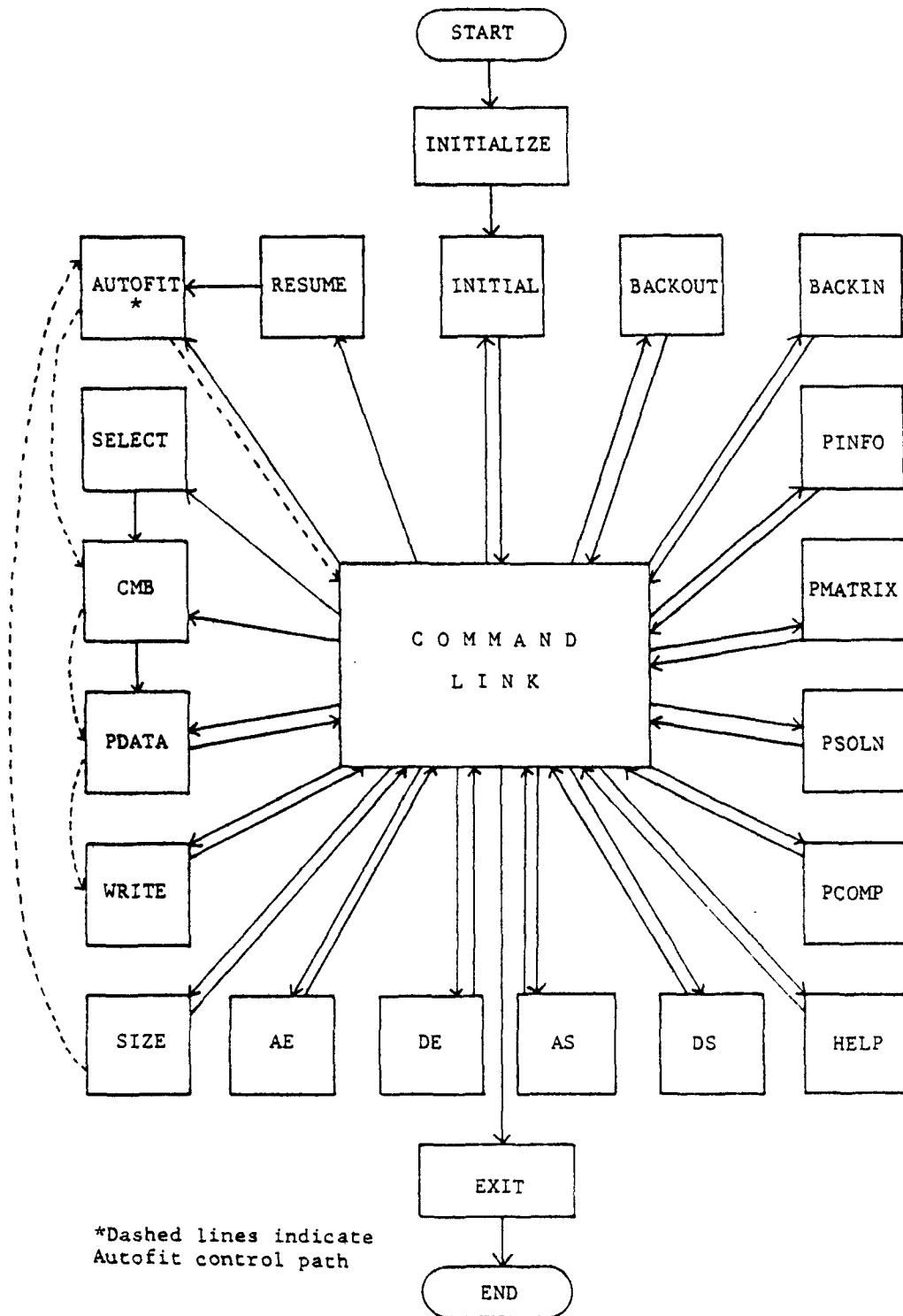


Figure B-1. Generalized Program Flow Diagram

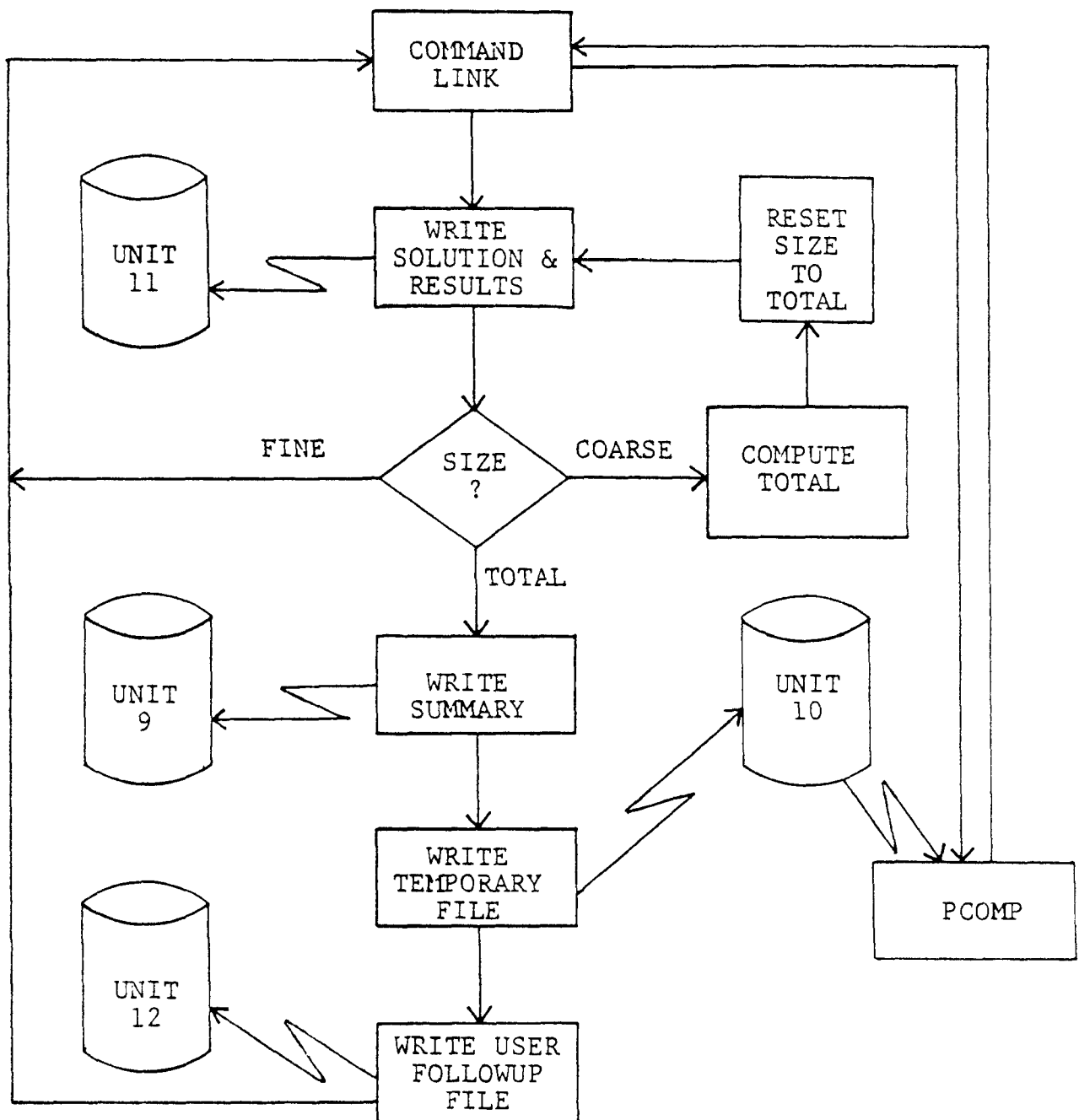


Figure B-2. WRITE Command Flow

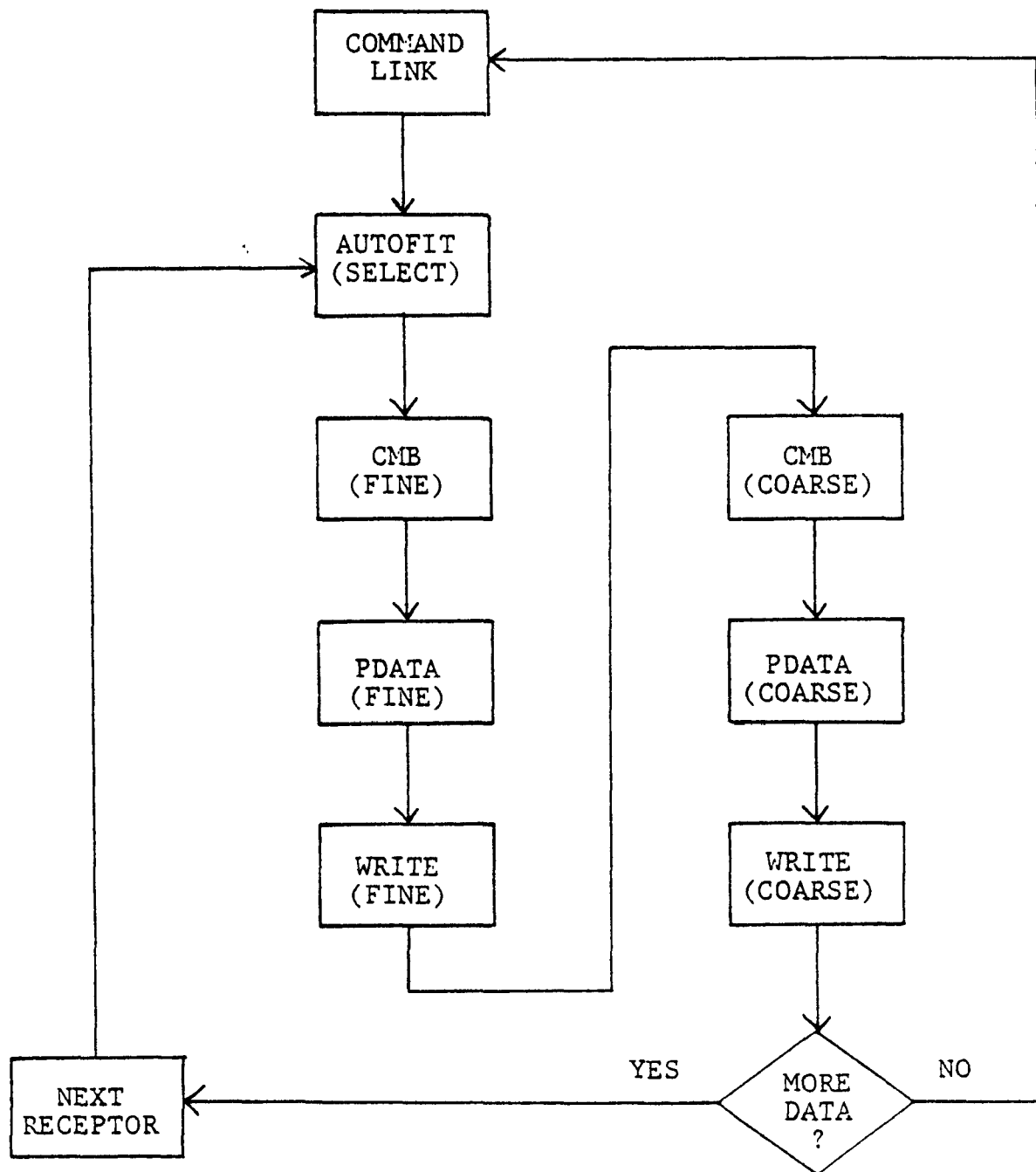


Figure B-3. AUTOFIT Command Flow

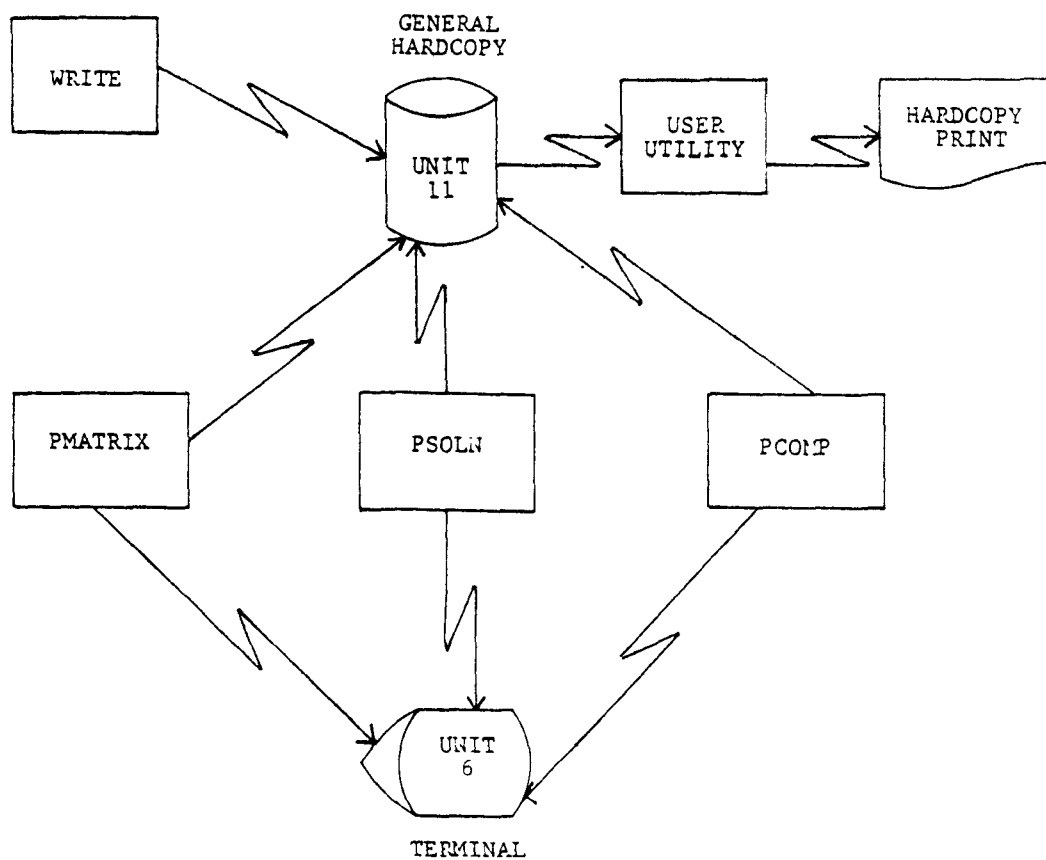


Figure B-4. General Hardcopy Communications

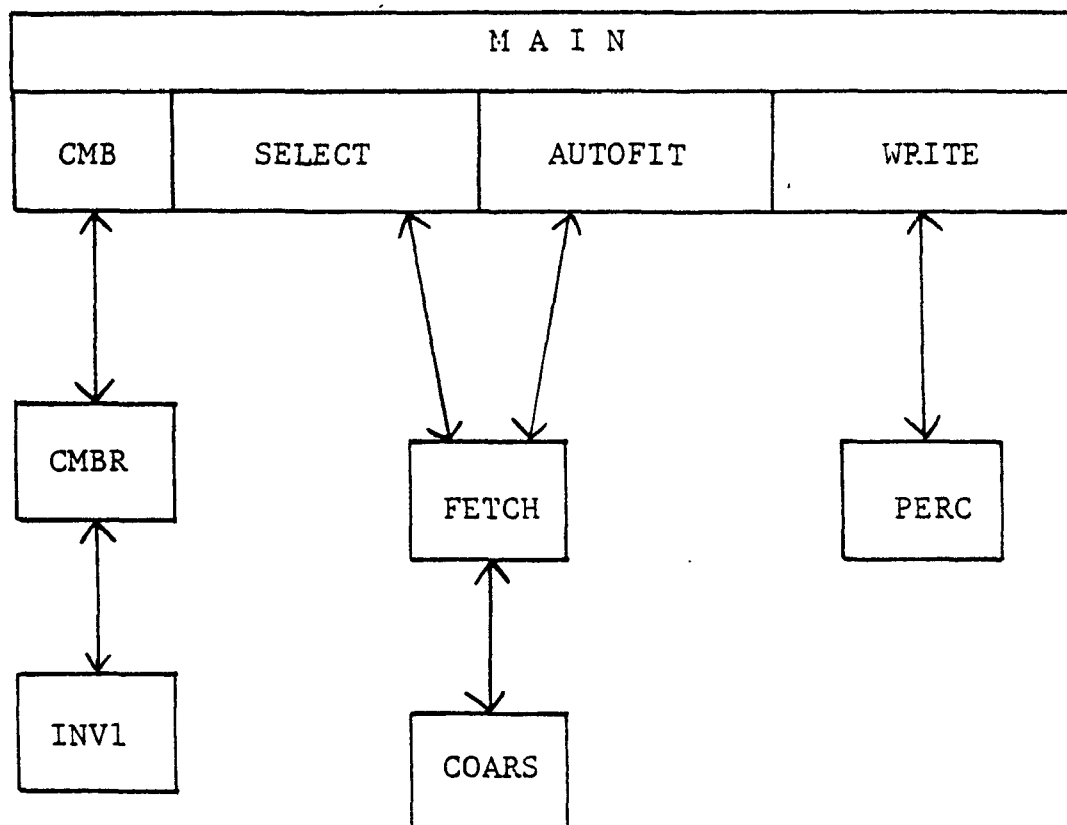
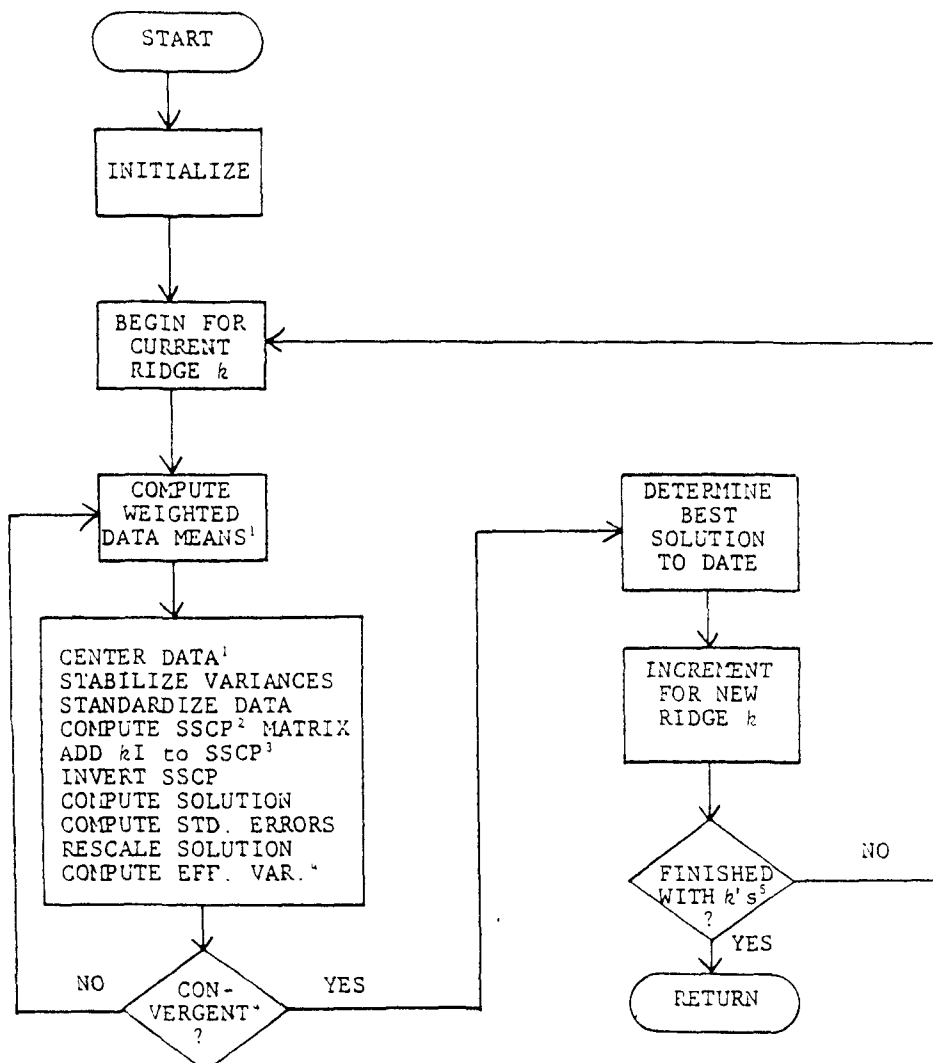


Figure B-5. Relationship of Main Program Commands and Subprogram Linkages



¹If intercept is called for.

²SSCP denotes sum of squares and cross products.

³I is the identity matrix.

⁴These items apply if the option to use effective variances is chosen.

⁵If ridge regression is not selected, 0 is the only value of k to be used.

Figure B-6. General CMBR Program Flow Diagram

APPENDIX C

INPUT AND OUTPUT FOR EXAMPLE RUN

This appendix contains example input and output file listings for the CMB program. The data given in Tables C-1 through C-5 are the input files used for the example interactive session of Section 4. The source signature data presented in Tables C-3 and C-4 were compiled by Dzubay and Hasan (1983). Accurate estimates of the standard errors are not currently available for all of the source signatures. A standard error of 25 percent of each source signature entry has been used strictly for illustrative purposes. The printouts given in Tables C-6, C-7, and C-8 are the output files from the interactive session.

TABLE C-1. SOURCE NAME AND CODE INPUT FILE

1	SOIL
2	RD DUST
3	SEA SALT
4	SLSH BRN
5	AUTO CAT
6	AUTO
7	JET AIR
8	RES OIL
9	DIST OIL
10	RES GAS
11	COAL
12	KRAFT RB
13	ELARCFRN
14	FERRMNFR
15	CAL GYP
16	CEMENT
17	PET FCC
18	LSKILN
19	SEC S04

TABLE C-2. SPECIES NAME AND CODE INPUT FILE

1	TOT
2	AL
3	AS
4	BA
5	BR
6	CA
7	CD
8	CL
9	CO
10	CR
11	CU
12	FE
13	HG
14	K
15	MN
16	NI
17	P
18	PB
19	SO4
20	SB
21	SI
22	SN
23	SR
24	TI
25	V
26	ZN
27	C
28	NA
29	NO3
30	RB
31	SE

TABLE C-3. FINE FRACTION SOURCE SIGNATURE INPUT FILE

1	2	.006500	.001625	AL	FINE SOIL
1	3	.000000	.000000	AS	FINE SOIL
1	4	.000000	.000000	BA	FINE SOIL
1	5	.000000	.000000	BR	FINE SOIL
1	27	.000000	.000000	C	FINE SOIL
1	6	.093000	.023250	CA	FINE SOIL
1	7	.000000	.000000	CD	FINE SOIL
1	8	.000000	.000000	CL	FINE SOIL
1	10	.000000	.000000	CR	FINE SOIL
1	11	.000300	.000075	CU	FINE SOIL
1	12	.008300	.002075	FE	FINE SOIL
1	14	.002000	.000500	K	FINE SOIL
1	15	.000370	.000093	MN	FINE SOIL
1	28	.000000	.000000	NA	FINE SOIL
1	16	.000000	.000000	NI	FINE SOIL
1	29	.000000	.000000	NO3	FINE SOIL
1	18	.000140	.000035	PB	FINE SOIL
1	30	.000020	.000005	RB	FINE SOIL
1	20	.000000	.000000	SB	FINE SOIL
1	31	.000000	.000000	SE	FINE SOIL
1	21	.024000	.006000	SI	FINE SOIL
1	22	.000000	.000000	SN	FINE SOIL
1	19	.004500	.001125	SO4	FINE SOIL
1	23	.000280	.000070	SR	FINE SOIL
1	24	.001400	.000350	TI	FINE SOIL
1	25	.000000	.000000	V	FINE SOIL
1	26	.000220	.000055	ZN	FINE SOIL
2	2	.088400	.022100	AL	FINE RD DUST
2	3	.000000	.000000	AS	FINE RD DUST
2	4	.000000	.000000	BA	FINE RD DUST
2	5	.000200	.000050	BR	FINE RD DUST
2	27	.136500	.034125	C	FINE RD DUST
2	6	.024400	.006100	CA	FINE RD DUST
2	7	.000000	.000000	CD	FINE RD DUST
2	8	.000000	.000000	CL	FINE RD DUST
2	10	.000450	.000112	CR	FINE RD DUST
2	11	.000300	.000075	CU	FINE RD DUST
2	12	.060000	.015000	FE	FINE RD DUST
2	14	.010300	.002575	K	FINE RD DUST
2	15	.001230	.000307	MN	FINE RD DUST
2	28	.012500	.003125	NA	FINE RD DUST
2	16	.000090	.000022	NI	FINE RD DUST
2	29	.000000	.000000	NO3	FINE RD DUST
2	18	.003700	.000925	PB	FINE RD DUST

TABLE C-3 (CONTINUED)

2	30	.000000	.000000	RB	FINE RD DUST
2	20	.000000	.000000	SB	FINE RD DUST
2	31	.000000	.000000	SE	FINE RD DUST
2	21	.223000	.055750	SI	FINE RD DUST
2	22	.000000	.000000	SN	FINE RD DUST
2	19	.011100	.002775	SO4	FINE RD DUST
2	23	.000000	.000000	SR	FINE RD DUST
2	24	.006400	.001600	TI	FINE RD DUST
2	25	.000230	.000057	V	FINE RD DUST
2	26	.001100	.000275	ZN	FINE RD DUST
3	2	.000000	.000000	AL	FINE SEA SALT
3	3	.000000	.000000	AS	FINE SEA SALT
3	4	.000000	.000000	BA	FINE SEA SALT
3	5	.000000	.000000	BR	FINE SEA SALT
3	27	.000000	.000000	C	FINE SEA SALT
3	6	.010000	.002500	CA	FINE SEA SALT
3	7	.000000	.000000	CD	FINE SEA SALT
3	8	.550000	.137500	CL	FINE SEA SALT
3	10	.000000	.000000	CR	FINE SEA SALT
3	11	.000000	.000000	CU	FINE SEA SALT
3	12	.000000	.000000	FE	FINE SEA SALT
3	14	.010000	.002500	K	FINE SEA SALT
3	15	.000000	.000000	MN	FINE SEA SALT
3	28	.310000	.077500	NA	FINE SEA SALT
3	16	.000000	.000000	NI	FINE SEA SALT
3	29	.000000	.000000	NO3	FINE SEA SALT
3	18	.000000	.000000	PB	FINE SEA SALT
3	30	.000000	.000000	RB	FINE SEA SALT
3	20	.000000	.000000	SB	FINE SEA SALT
3	31	.000000	.000000	SE	FINE SEA SALT
3	21	.000000	.000000	SI	FINE SEA SALT
3	22	.000000	.000000	SN	FINE SEA SALT
3	19	.090000	.022500	SO4	FINE SEA SALT
3	23	.000000	.000000	SR	FINE SEA SALT
3	24	.000000	.000000	TI	FINE SEA SALT
3	25	.000000	.000000	V	FINE SEA SALT
3	26	.000000	.000000	ZN	FINE SEA SALT
4	2	.014400	.003600	AL	FINE SLASH BURN
4	3	.000000	.000000	AS	FINE SLASH BURN
4	4	.000530	.000132	BA	FINE SLASH BURN
4	5	.000530	.000132	BR	FINE SLASH BURN
4	27	.629000	.157250	C	FINE SLASH BURN
4	6	.010700	.002675	CA	FINE SLASH BURN
4	7	.000530	.000132	CD	FINE SLASH BURN
4	8	.055500	.013875	CL	FINE SLASH BURN
4	10	.000000	.000000	CR	FINE SLASH BURN
4	11	.000900	.000225	CU	FINE SLASH BURN

TABLE C-3 (CONTINUED)

4	12	.001900	.000475	FE	FINE SLASH BURN
4	14	.006000	.001500	K	FINE SLASH BURN
4	15	.001200	.000300	MN	FINE SLASH BURN
4	28	.006500	.001625	NA	FINE SLASH BURN
4	16	.000000	.000000	NI	FINE SLASH BURN
4	29	.051000	.012750	NO3	FINE SLASH BURN
4	18	.000530	.000132	PB	FINE SLASH BURN
4	30	.000530	.000132	RB	FINE SLASH BURN
4	20	.000530	.000132	SB	FINE SLASH BURN
4	31	.000000	.000000	SE	FINE SLASH BURN
4	21	.008900	.002225	SI	FINE SLASH BURN
4	22	.000530	.000132	SN	FINE SLASH BURN
4	19	.016000	.004000	SO4	FINE SLASH BURN
4	23	.000530	.000132	SR	FINE SLASH BURN
4	24	.000000	.000000	TI	FINE SLASH BURN
4	25	.000000	.000000	V	FINE SLASH BURN
4	26	.000000	.000000	ZN	FINE SLASH BURN
5	2	.001200	.000300	AL	FINE AUTO W CAT
5	3	.000000	.000000	AS	FINE AUTO W CAT
5	4	.000000	.000000	BA	FINE AUTO W CAT
5	5	.000000	.000000	BR	FINE AUTO W CAT
5	27	.390000	.097500	C	FINE AUTO W CAT
5	6	.001700	.000425	CA	FINE AUTO W CAT
5	7	.000000	.000000	CD	FINE AUTO W CAT
5	8	.000000	.000000	CL	FINE AUTO W CAT
5	10	.000000	.000000	CR	FINE AUTO W CAT
5	11	.000240	.000060	CU	FINE AUTO W CAT
5	12	.001100	.000275	FE	FINE AUTO W CAT
5	14	.000440	.000110	K	FINE AUTO W CAT
5	15	.000150	.000037	MN	FINE AUTO W CAT
5	28	.000000	.000000	NA	FINE AUTO W CAT
5	16	.000150	.000037	NI	FINE AUTO W CAT
5	29	.000000	.000000	NO3	FINE AUTO W CAT
5	18	.000000	.000000	PB	FINE AUTO W CAT
5	30	.000000	.000000	RB	FINE AUTO W CAT
5	20	.000000	.000000	SB	FINE AUTO W CAT
5	31	.000000	.000000	SE	FINE AUTO W CAT
5	21	.005100	.001275	SI	FINE AUTO W CAT
5	22	.000000	.000000	SN	FINE AUTO W CAT
5	19	.500000	.125000	SO4	FINE AUTO W CAT
5	23	.000000	.000000	SR	FINE AUTO W CAT
5	24	.000000	.000000	TI	FINE AUTO W CAT
5	25	.000000	.000000	V	FINE AUTO W CAT
5	26	.000800	.000200	ZN	FINE AUTO W CAT
6	2	.000430	.000108	AL	FINE AUTO
6	3	.000000	.000000	AS	FINE AUTO

TABLE C-3 (CONTINUED)

6	4	.000000	.000000	BA	FINE AUTO
6	5	.082000	.020500	BR	FINE AUTO
6	27	.545000	.136250	C	FINE AUTO
6	6	.000000	.000000	CA	FINE AUTO
6	7	.000000	.000000	CD	FINE AUTO
6	8	.054000	.013500	CL	FINE AUTO
6	10	.000000	.000000	CR	FINE AUTO
6	11	.000040	.000010	CU	FINE AUTO
6	12	.002500	.000625	FE	FINE AUTO
6	14	.000000	.000000	K	FINE AUTO
6	15	.000000	.000000	MN	FINE AUTO
6	28	.000000	.000000	NA	FINE AUTO
6	16	.000000	.000000	NI	FINE AUTO
6	29	.000000	.000000	NO3	FINE AUTO
6	18	.211000	.052750	PB	FINE AUTO
6	30	.000000	.000000	RB	FINE AUTO
6	20	.000000	.000000	SB	FINE AUTO
6	31	.000000	.000000	SE	FINE AUTO
6	21	.000750	.000187	SI	FINE AUTO
6	22	.000000	.000000	SN	FINE AUTO
6	19	.002100	.000525	SO4	FINE AUTO
6	23	.000000	.000000	SR	FINE AUTO
6	24	.000000	.000000	TI	FINE AUTO
6	25	.000000	.000000	V	FINE AUTO
6	26	.000210	.000053	ZN	FINE AUTO
7	2	.000000	.000000	AL	FINE JET AIR
7	3	.000000	.000000	AS	FINE JET AIR
7	4	.000000	.000000	BA	FINE JET AIR
7	5	.000000	.000000	BR	FINE JET AIR
7	27	.960000	.240000	C	FINE JET AIR
7	6	.000000	.000000	CA	FINE JET AIR
7	7	.000000	.000000	CD	FINE JET AIR
7	8	.000000	.000000	CL	FINE JET AIR
7	10	.000000	.000000	CR	FINE JET AIR
7	11	.000000	.000000	CU	FINE JET AIR
7	12	.000000	.000000	FE	FINE JET AIR
7	14	.000000	.000000	K	FINE JET AIR
7	15	.000000	.000000	MN	FINE JET AIR
7	28	.000000	.000000	NA	FINE JET AIR
7	16	.000000	.000000	NI	FINE JET AIR
7	29	.000000	.000000	NO3	FINE JET AIR
7	18	.000000	.000000	PB	FINE JET AIR
7	30	.000000	.000000	RB	FINE JET AIR
7	20	.000000	.000000	SB	FINE JET AIR
7	31	.000000	.000000	SE	FINE JET AIR
7	21	.000000	.000000	SI	FINE JET AIR

TABLE C-3 (CONTINUED)

7	22	.000000	.000000	SN	FINE JET AIR
7	19	.000000	.000000	SO4	FINE JET AIR
7	23	.000000	.000000	SR	FINE JET AIR
7	24	.000000	.000000	TI	FINE JET AIR
7	25	.000000	.000000	V	FINE JET AIR
7	26	.000000	.000000	ZN	FINE JET AIR
8	2	.005300	.001325	AL	FINE RESIDUAL OIL
8	3	.000000	.000000	AS	FINE RESIDUAL OIL
8	4	.000000	.000000	BA	FINE RESIDUAL OIL
8	5	.000130	.000033	BR	FINE RESIDUAL OIL
8	27	.101000	.025250	C	FINE RESIDUAL OIL
8	6	.015800	.003950	CA	FINE RESIDUAL OIL
8	7	.000000	.000000	CD	FINE RESIDUAL OIL
8	8	.000000	.000000	CL	FINE RESIDUAL OIL
8	10	.000470	.000117	CR	FINE RESIDUAL OIL
8	11	.000750	.000187	CU	FINE RESIDUAL OIL
8	12	.029700	.007425	FE	FINE RESIDUAL OIL
8	14	.002800	.000700	K	FINE RESIDUAL OIL
8	15	.000460	.000115	MN	FINE RESIDUAL OIL
8	28	.035000	.008750	NA	FINE RESIDUAL OIL
8	16	.053600	.013400	NI	FINE RESIDUAL OIL
8	29	.006500	.001625	NO3	FINE RESIDUAL OIL
8	18	.001100	.000275	PB	FINE RESIDUAL OIL
8	30	.000000	.000000	RB	FINE RESIDUAL OIL
8	20	.000000	.000000	SB	FINE RESIDUAL OIL
8	31	.000000	.000000	SE	FINE RESIDUAL OIL
8	21	.009600	.002400	SI	FINE RESIDUAL OIL
8	22	.000000	.000000	SN	FINE RESIDUAL OIL
8	19	.481000	.120250	SO4	FINE RESIDUAL OIL
8	23	.000000	.000000	SR	FINE RESIDUAL OIL
8	24	.001100	.000275	TI	FINE RESIDUAL OIL
8	25	.034400	.008600	V	FINE RESIDUAL OIL
8	26	.004000	.001000	ZN	FINE RESIDUAL OIL
9	2	.003100	.000775	AL	FINE DISTILLATE OIL
9	3	.000000	.000000	AS	FINE DISTILLATE OIL
9	4	.000000	.000000	BA	FINE DISTILLATE OIL
9	5	.000260	.000065	BR	FINE DISTILLATE OIL
9	27	.358000	.089500	C	FINE DISTILLATE OIL
9	6	.005000	.001250	CA	FINE DISTILLATE OIL
9	7	.000000	.000000	CD	FINE DISTILLATE OIL
9	8	.012000	.003000	CL	FINE DISTILLATE OIL
9	10	.000000	.000000	CR	FINE DISTILLATE OIL
9	11	.001700	.000425	CU	FINE DISTILLATE OIL
9	12	.001200	.000300	FE	FINE DISTILLATE OIL
9	14	.000180	.000045	K	FINE DISTILLATE OIL
9	15	.000140	.000035	MN	FINE DISTILLATE OIL
9	28	.003200	.000800	NA	FINE DISTILLATE OIL

TABLE C-3 (CONTINUED)

9	16	.000090	.000022	NI	FINE DISTILLATE OIL
9	29	.010000	.002500	NO3	FINE DISTILLATE OIL
9	18	.005400	.001350	PB	FINE DISTILLATE OIL
9	30	.000000	.000000	RB	FINE DISTILLATE OIL
9	20	.000000	.000000	SB	FINE DISTILLATE OIL
9	31	.000000	.000000	SE	FINE DISTILLATE OIL
9	21	.002700	.000675	SI	FINE DISTILLATE OIL
9	22	.000000	.000000	SN	FINE DISTILLATE OIL
9	19	.132000	.033000	SO4	FINE DISTILLATE OIL
9	23	.000000	.000000	SR	FINE DISTILLATE OIL
9	24	.000000	.000000	TI	FINE DISTILLATE OIL
9	25	.000050	.000013	V	FINE DISTILLATE OIL
9	26	.000290	.000072	ZN	FINE DISTILLATE OIL
10	2	.000000	.000000	AL	FINE RESIDENTIAL GAS
10	3	.000000	.000000	AS	FINE RESIDENTIAL GAS
10	4	.000000	.000000	BA	FINE RESIDENTIAL GAS
10	5	.000000	.000000	BR	FINE RESIDENTIAL GAS
10	27	.120000	.030000	C	FINE RESIDENTIAL GAS
10	6	.050000	.012500	CA	FINE RESIDENTIAL GAS
10	7	.000000	.000000	CD	FINE RESIDENTIAL GAS
10	8	.000000	.000000	CL	FINE RESIDENTIAL GAS
10	10	.000000	.000000	CR	FINE RESIDENTIAL GAS
10	11	.000000	.000000	CU	FINE RESIDENTIAL GAS
10	12	.000000	.000000	FE	FINE RESIDENTIAL GAS
10	14	.000000	.000000	K	FINE RESIDENTIAL GAS
10	15	.000000	.000000	MN	FINE RESIDENTIAL GAS
10	28	.000000	.000000	NA	FINE RESIDENTIAL GAS
10	16	.000000	.000000	NI	FINE RESIDENTIAL GAS
10	29	.000000	.000000	NO3	FINE RESIDENTIAL GAS
10	18	.000000	.000000	PB	FINE RESIDENTIAL GAS
10	30	.000000	.000000	RB	FINE RESIDENTIAL GAS
10	20	.000000	.000000	SB	FINE RESIDENTIAL GAS
10	31	.000000	.000000	SE	FINE RESIDENTIAL GAS
10	21	.000000	.000000	SI	FINE RESIDENTIAL GAS
10	22	.000000	.000000	SN	FINE RESIDENTIAL GAS
10	19	.470000	.117500	SO4	FINE RESIDENTIAL GAS
10	23	.000000	.000000	SR	FINE RESIDENTIAL GAS
10	24	.000000	.000000	TI	FINE RESIDENTIAL GAS
10	25	.000000	.000000	V	FINE RESIDENTIAL GAS
10	26	.000000	.000000	ZN	FINE RESIDENTIAL GAS
11	2	.004380	.001095	AL	FINE COAL
11	3	.000000	.000000	AS	FINE COAL
11	4	.000120	.000030	BA	FINE COAL
11	5	.000000	.000000	BR	FINE COAL
11	27	.000000	.000000	C	FINE COAL
11	6	.018180	.004545	CA	FINE COAL
11	7	.000850	.000223	CD	FINE COAL

TABLE C-3 (CONTINUED)

11	8	.000000	.000000	CL	FINE COAL
11	10	.000160	.000040	CR	FINE COAL
11	11	.000210	.000053	CU	FINE COAL
11	12	.043330	.010832	FE	FINE COAL
11	14	.001890	.000472	K	FINE COAL
11	15	.000000	.000000	MN	FINE COAL
11	28	.002420	.000605	NA	FINE COAL
11	16	.000070	.000018	NI	FINE COAL
11	29	.000000	.000000	NO3	FINE COAL
11	18	.006690	.001673	PB	FINE COAL
11	30	.000000	.000000	RB	FINE COAL
11	20	.000290	.000072	SB	FINE COAL
11	31	.000000	.000000	SE	FINE COAL
11	21	.035550	.008888	SI	FINE COAL
11	22	.008240	.002060	SN	FINE COAL
11	19	.096290	.024072	SO4	FINE COAL
11	23	.000000	.000000	SR	FINE COAL
11	24	.001210	.000303	TI	FINE COAL
11	25	.000000	.000000	V	FINE COAL
11	26	.016270	.004068	ZN	FINE COAL
12	2	.002500	.000625	AL	KRAFT REC BOILER
12	3	.000000	.000000	AS	KRAFT REC BOILER
12	4	.000000	.000000	BA	KRAFT REC BOILER
12	5	.001300	.000325	BR	KRAFT REC BOILER
12	27	.019200	.004800	C	KRAFT REC BOILER
12	6	.000000	.000000	CA	KRAFT REC BOILER
12	7	.000000	.000000	CD	KRAFT REC BOILER
12	8	.018000	.004500	CL	KRAFT REC BOILER
12	10	.002800	.000700	CR	KRAFT REC BOILER
12	11	.000210	.000053	CU	KRAFT REC BOILER
12	12	.012000	.003000	FE	KRAFT REC BOILER
12	14	.015000	.003750	K	KRAFT REC BOILER
12	15	.000300	.000075	MN	KRAFT REC BOILER
12	28	.127000	.031750	NA	KRAFT REC BOILER
12	16	.001400	.000350	NI	KRAFT REC BOILER
12	29	.000000	.000000	NO3	KRAFT REC BOILER
12	18	.000130	.000033	PB	KRAFT REC BOILER
12	30	.000000	.000000	RB	KRAFT REC BOILER
12	20	.000000	.000000	SB	KRAFT REC BOILER
12	31	.000000	.000000	SE	KRAFT REC BOILER
12	21	.001500	.000375	SI	KRAFT REC BOILER
12	22	.000000	.000000	SN	KRAFT REC BOILER
12	19	.400000	.100000	SO4	KRAFT REC BOILER
12	23	.000000	.000000	SR	KRAFT REC BOILER
12	24	.000060	.000015	TI	KRAFT REC BOILER
12	25	.000010	.000002	V	KRAFT REC BOILER
12	26	.000690	.000173	ZN	KRAFT REC BOILER

TABLE C-3 (CONTINUED)

13	2	.006500	.001625	AL	FINE ELECTRIC ARC FURN
13	3	.000000	.000000	AS	FINE ELECTRIC ARC FURN
13	4	.000000	.000000	BA	FINE ELECTRIC ARC FURN
13	5	.000000	.000000	BR	FINE ELECTRIC ARC FURN
13	27	.000000	.000000	C	FINE ELECTRIC ARC FURN
13	6	.062000	.015500	CA	FINE ELECTRIC ARC FURN
13	7	.000000	.000000	CD	FINE ELECTRIC ARC FURN
13	8	.018500	.004625	CL	FINE ELECTRIC ARC FURN
13	10	.021000	.005250	CR	FINE ELECTRIC ARC FURN
13	11	.002800	.000700	CU	FINE ELECTRIC ARC FURN
13	12	.319500	.079875	FE	FINE ELECTRIC ARC FURN
13	14	.009200	.002300	K	FINE ELECTRIC ARC FURN
13	15	.087000	.021750	MN	FINE ELECTRIC ARC FURN
13	28	.012600	.003150	NA	FINE ELECTRIC ARC FURN
13	16	.007100	.001775	NI	FINE ELECTRIC ARC FURN
13	29	.000000	.000000	NO3	FINE ELECTRIC ARC FURN
13	18	.007600	.001900	PB	FINE ELECTRIC ARC FURN
13	30	.000000	.000000	RB	FINE ELECTRIC ARC FURN
13	20	.000000	.000000	SB	FINE ELECTRIC ARC FURN
13	31	.000000	.000000	SE	FINE ELECTRIC ARC FURN
13	21	.050000	.012500	SI	FINE ELECTRIC ARC FURN
13	22	.000000	.000000	SN	FINE ELECTRIC ARC FURN
13	19	.025000	.006250	SO4	FINE ELECTRIC ARC FURN
13	23	.000000	.000000	SR	FINE ELECTRIC ARC FURN
13	24	.002000	.000500	TI	FINE ELECTRIC ARC FURN
13	25	.000630	.000158	V	FINE ELECTRIC ARC FURN
13	26	.012000	.003000	ZN	FINE ELECTRIC ARC FURN
14	2	.006400	.001600	AL	FINE FERROMANGANESE FURN
14	3	.000000	.000000	AS	FINE FERROMANGANESE FURN
14	4	.000000	.000000	BA	FINE FERROMANGANESE FURN
14	5	.001600	.000400	BR	FINE FERROMANGANESE FURN
14	27	.105000	.026250	C	FINE FERROMANGANESE FURN
14	6	.013000	.003250	CA	FINE FERROMANGANESE FURN
14	7	.000000	.000000	CD	FINE FERROMANGANESE FURN
14	8	.004200	.001050	CL	FINE FERROMANGANESE FURN
14	10	.000420	.000105	CR	FINE FERROMANGANESE FURN
14	11	.000360	.000090	CU	FINE FERROMANGANESE FURN
14	12	.021000	.005250	FE	FINE FERROMANGANESE FURN
14	14	.105000	.026250	K	FINE FERROMANGANESE FURN
14	15	.173000	.043250	MN	FINE FERROMANGANESE FURN
14	28	.031000	.007750	NA	FINE FERROMANGANESE FURN
14	16	.000000	.000000	NI	FINE FERROMANGANESE FURN
14	29	.057000	.014250	NO3	FINE FERROMANGANESE FURN
14	18	.000450	.000112	PB	FINE FERROMANGANESE FURN
14	30	.000000	.000000	RB	FINE FERROMANGANESE FURN

TABLE C-3 (CONTINUED)

14	20	.000000	.000000	SB	FINE FERROMANGANESE FURN
14	31	.000000	.000000	SE	FINE FERROMANGANESE FURN
14	21	.009900	.002475	SI	FINE FERROMANGANESE FURN
14	22	.000000	.000000	SN	FINE FERROMANGANESE FURN
14	19	.042000	.010500	SO4	FINE FERROMANGANESE FURN
14	23	.000000	.000000	SR	FINE FERROMANGANESE FURN
14	24	.000460	.000115	TI	FINE FERROMANGANESE FURN
14	25	.000240	.000060	V	FINE FERROMANGANESE FURN
14	26	.005800	.001450	ZN	FINE FERROMANGANESE FURN
15	2	.000000	.000000	AL	FINE CALCINAION OF GYPSUM
15	3	.000000	.000000	AS	FINE CALCINAION OF GYPSUM
15	4	.000000	.000000	BA	FINE CALCINAION OF GYPSUM
15	5	.000000	.000000	BR	FINE CALCINAION OF GYPSUM
15	27	.010000	.002500	C	FINE CALCINAION OF GYPSUM
15	6	.130000	.032500	CA	FINE CALCINAION OF GYPSUM
15	7	.000000	.000000	CD	FINE CALCINAION OF GYPSUM
15	8	.000000	.000000	CL	FINE CALCINAION OF GYPSUM
15	10	.000000	.000000	CR	FINE CALCINAION OF GYPSUM
15	11	.000000	.000000	CU	FINE CALCINAION OF GYPSUM
15	12	.000000	.000000	FE	FINE CALCINAION OF GYPSUM
15	14	.000000	.000000	K	FINE CALCINAION OF GYPSUM
15	15	.000000	.000000	MN	FINE CALCINAION OF GYPSUM
15	28	.000000	.000000	NA	FINE CALCINAION OF GYPSUM
15	16	.000000	.000000	NI	FINE CALCINAION OF GYPSUM
15	29	.000000	.000000	NO3	FINE CALCINAION OF GYPSUM
15	18	.000000	.000000	PB	FINE CALCINAION OF GYPSUM
15	30	.000000	.000000	RB	FINE CALCINAION OF GYPSUM
15	20	.000000	.000000	SB	FINE CALCINAION OF GYPSUM
15	31	.000000	.000000	SE	FINE CALCINAION OF GYPSUM
15	21	.000000	.000000	SI	FINE CALCINAION OF GYPSUM
15	22	.000000	.000000	SN	FINE CALCINAION OF GYPSUM
15	19	.410000	.102500	SO4	FINE CALCINAION OF GYPSUM
15	23	.000000	.000000	SR	FINE CALCINAION OF GYPSUM
15	24	.000000	.000000	TI	FINE CALCINAION OF GYPSUM
15	25	.000000	.000000	V	FINE CALCINAION OF GYPSUM
15	26	.000000	.000000	ZN	FINE CALCINAION OF GYPSUM
16	2	.000000	.000000	AL	FINE CEMENT
16	3	.000000	.000000	AS	FINE CEMENT
16	4	.000000	.000000	BA	FINE CEMENT
16	5	.000000	.000000	BR	FINE CEMENT
16	27	.080000	.020000	C	FINE CEMENT
16	6	.050000	.012500	CA	FINE CEMENT
16	7	.000000	.000000	CD	FINE CEMENT
16	8	.000000	.000000	CL	FINE CEMENT
16	10	.000000	.000000	CR	FINE CEMENT
16	11	.000000	.000000	CU	FINE CEMENT

TABLE C-3 (CONTINUED)

16	12	.000000	.000000	FE	FINE CEMENT
16	14	.020000	.005000	K	FINE CEMENT
16	15	.000000	.000000	MN	FINE CEMENT
16	28	.000000	.000000	NA	FINE CEMENT
16	16	.000000	.000000	NI	FINE CEMENT
16	29	.000000	.000000	NO3	FINE CEMENT
16	18	.000000	.000000	PB	FINE CEMENT
16	30	.000000	.000000	RB	FINE CEMENT
16	20	.000000	.000000	SB	FINE CEMENT
16	31	.000000	.000000	SE	FINE CEMENT
16	21	.025000	.006250	SI	FINE CEMENT
16	22	.000000	.000000	SN	FINE CEMENT
16	19	.600000	.150000	SO4	FINE CEMENT
16	23	.000000	.000000	SR	FINE CEMENT
16	24	.000000	.000000	TI	FINE CEMENT
16	25	.000000	.000000	V	FINE CEMENT
16	26	.000000	.000000	ZN	FINE CEMENT
17	2	.000000	.000000	AL	FINE PETROL FCC UNITS
17	3	.000000	.000000	AS	FINE PETROL FCC UNITS
17	4	.000000	.000000	BA	FINE PETROL FCC UNITS
17	5	.000000	.000000	BR	FINE PETROL FCC UNITS
17	27	.040000	.010000	C	FINE PETROL FCC UNITS
17	6	.000000	.000000	CA	FINE PETROL FCC UNITS
17	7	.000000	.000000	CD	FINE PETROL FCC UNITS
17	8	.000000	.000000	CL	FINE PETROL FCC UNITS
17	10	.000000	.000000	CR	FINE PETROL FCC UNITS
17	11	.000000	.000000	CU	FINE PETROL FCC UNITS
17	12	.010000	.002500	FE	FINE PETROL FCC UNITS
17	14	.000000	.000000	K	FINE PETROL FCC UNITS
17	15	.000000	.000000	MN	FINE PETROL FCC UNITS
17	28	.000000	.000000	NA	FINE PETROL FCC UNITS
17	16	.000000	.000000	NI	FINE PETROL FCC UNITS
17	29	.000000	.000000	NO3	FINE PETROL FCC UNITS
17	18	.000000	.000000	PB	FINE PETROL FCC UNITS
17	30	.000000	.000000	RB	FINE PETROL FCC UNITS
17	20	.000000	.000000	SB	FINE PETROL FCC UNITS
17	31	.000000	.000000	SE	FINE PETROL FCC UNITS
17	21	.000000	.000000	SI	FINE PETROL FCC UNITS
17	22	.000000	.000000	SN	FINE PETROL FCC UNITS
17	19	.500000	.125000	SO4	FINE PETROL FCC UNITS
17	23	.000000	.000000	SR	FINE PETROL FCC UNITS
17	24	.000000	.000000	TI	FINE PETROL FCC UNITS
17	25	.000000	.000000	V	FINE PETROL FCC UNITS
17	26	.000000	.000000	ZN	FINE PETROL FCC UNITS
18	2	.000000	.000000	AL	FINE LS KILN

TABLE C-3 (CONTINUED)

18	3	.000000	.000000	AS	FINE LS KILN
18	4	.000000	.000000	BA	FINE LS KILN
18	5	.000000	.000000	BR	FINE LS KILN
18	27	.400000	.100000	C	FINE LS KILN
18	6	.300000	.075000	CA	FINE LS KILN
18	7	.000000	.000000	CD	FINE LS KILN
18	8	.000000	.000000	CL	FINE LS KILN
18	10	.000000	.000000	CR	FINE LS KILN
18	11	.000000	.000000	CU	FINE LS KILN
18	12	.020000	.005000	FE	FINE LS KILN
18	14	.000000	.000000	K	FINE LS KILN
18	15	.000000	.000000	MN	FINE LS KILN
18	28	.000000	.000000	NA	FINE LS KILN
18	16	.000000	.000000	NI	FINE LS KILN
18	29	.000000	.000000	NO3	FINE LS KILN
18	18	.000000	.000000	PB	FINE LS KILN
18	30	.000000	.000000	RB	FINE LS KILN
18	20	.000000	.000000	SB	FINE LS KILN
18	31	.100000	.025000	SE	FINE LS KILN
18	21	.000000	.000000	SI	FINE LS KILN
18	22	.000000	.000000	SN	FINE LS KILN
18	19	.000000	.000000	SO4	FINE LS KILN
18	23	.000000	.000000	SR	FINE LS KILN
18	24	.000000	.000000	TI	FINE LS KILN
18	25	.000000	.000000	V	FINE LS KILN
18	26	.000000	.000000	ZN	FINE LS KILN
19	2	.000000	.000000	AL	FINE SEC SO4
19	3	.000000	.000000	AS	FINE SEC SO4
19	4	.000000	.000000	BA	FINE SEC SO4
19	5	.000000	.000000	BR	FINE SEC SO4
19	27	.000000	.000000	C	FINE SEC SO4
19	6	.000000	.000000	CA	FINE SEC SO4
19	7	.000000	.000000	CD	FINE SEC SO4
19	8	.000000	.000000	CL	FINE SEC SO4
19	10	.000000	.000000	CR	FINE SEC SO4
19	11	.000000	.000000	CU	FINE SEC SO4
19	12	.000000	.000000	FE	FINE SEC SO4
19	14	.000000	.000000	K	FINE SEC SO4
19	15	.000000	.000000	MN	FINE SEC SO4
19	28	.000000	.000000	NA	FINE SEC SO4
19	16	.000000	.000000	NI	FINE SEC SO4
19	29	.000000	.000000	NO3	FINE SEC SO4
19	18	.000000	.000000	PB	FINE SEC SO4
19	30	.000000	.000000	RB	FINE SEC SO4
19	20	.000000	.000000	SB	FINE SEC SO4

TABLE C-3 (CONTINUED)

19	31	.000000	.000000	SE	FINE SEC S04
19	21	.000000	.000000	SI	FINE SEC S04
19	22	.000000	.000000	SN	FINE SEC S04
19	19	1.000000	.000000	S04	FINE SEC S04
19	23	.000000	.000000	SR	FINE SEC S04
19	24	.000000	.000000	TI	FINE SEC S04
19	25	.000000	.000000	V	FINE SEC S04
19	26	.000000	.000000	ZN	FINE SEC S04

TABLE C-4. COARSE FRACTION SOURCE SIGNATURE INPUT FILE

1	2	.005500	.001375	AL	COARSE SOIL
1	3	.000000	.000000	AS	COARSE SOIL
1	4	.000000	.000000	BA	COARSE SOIL
1	5	.000000	.000000	BR	COARSE SOIL
1	27	.000000	.000000	C	COARSE SOIL
1	6	.051000	.012750	CA	COARSE SOIL
1	7	.000000	.000000	CD	COARSE SOIL
1	8	.000000	.000000	CL	COARSE SOIL
1	10	.000000	.000000	CR	COARSE SOIL
1	11	.000090	.000022	CU	COARSE SOIL
1	12	.004800	.001200	FE	COARSE SOIL
1	14	.001200	.000300	K	COARSE SOIL
1	15	.000210	.000053	MN	COARSE SOIL
1	28	.000000	.000000	NA	COARSE SOIL
1	16	.000000	.000000	NI	COARSE SOIL
1	29	.000000	.000000	NO3	COARSE SOIL
1	18	.000200	.000050	PB	COARSE SOIL
1	30	.000020	.000005	RB	COARSE SOIL
1	20	.000000	.000000	SB	COARSE SOIL
1	31	.000000	.000000	SE	COARSE SOIL
1	21	.024000	.006000	SI	COARSE SOIL
1	22	.000000	.000000	SN	COARSE SOIL
1	19	.002700	.000675	SO4	COARSE SOIL
1	23	.000140	.000035	SR	COARSE SOIL
1	24	.000890	.000223	TI	COARSE SOIL
1	25	.000000	.000000	V	COARSE SOIL
1	26	.000090	.000022	ZN	COARSE SOIL
2	2	.065900	.016475	AL	COARSE RD DUST
2	3	.000000	.000000	AS	COARSE RD DUST
2	4	.000000	.000000	BA	COARSE RD DUST
2	5	.000080	.000020	BR	COARSE RD DUST
2	27	.048900	.012225	C	COARSE RD DUST
2	6	.030000	.007500	CA	COARSE RD DUST
2	7	.000000	.000000	CD	COARSE RD DUST
2	8	.000000	.000000	CL	COARSE RD DUST
2	10	.000000	.000000	CR	COARSE RD DUST
2	11	.000000	.000000	CU	COARSE RD DUST
2	12	.057300	.014325	FE	COARSE RD DUST
2	14	.000000	.000000	K	COARSE RD DUST
2	15	.001000	.000250	MN	COARSE RD DUST
2	28	.017500	.004375	NA	COARSE RD DUST
2	16	.000000	.000000	NI	COARSE RD DUST
2	29	.000200	.000050	NO3	COARSE RD DUST
2	18	.000000	.000000	PB	COARSE RD DUST

TABLE C-4 (CONTINUED)

2	30	.000000	.000000	RB	COARSE RD DUST
2	20	.000000	.000000	SB	COARSE RD DUST
2	31	.000000	.000000	SE	COARSE RD DUST
2	21	.284000	.071000	SI	COARSE RD DUST
2	22	.000000	.000000	SN	COARSE RD DUST
2	19	.000000	.000000	SO4	COARSE RD DUST
2	23	.000000	.000000	SR	COARSE RD DUST
2	24	.010100	.002525	TI	COARSE RD DUST
2	25	.000270	.000068	V	COARSE RD DUST
2	26	.000000	.000000	ZN	COARSE RD DUST
3	2	.000000	.000000	AL	COARSE SEA SALT
3	3	.000000	.000000	AS	COARSE SEA SALT
3	4	.000000	.000000	BA	COARSE SEA SALT
3	5	.000000	.000000	BR	COARSE SEA SALT
3	27	.000000	.000000	C	COARSE SEA SALT
3	6	.010000	.002500	CA	COARSE SEA SALT
3	7	.000000	.000000	CD	COARSE SEA SALT
3	8	.550000	.137500	CL	COARSE SEA SALT
3	10	.000000	.000000	CR	COARSE SEA SALT
3	11	.000000	.000000	CU	COARSE SEA SALT
3	12	.000000	.000000	FE	COARSE SEA SALT
3	14	.010000	.002500	K	COARSE SEA SALT
3	15	.000000	.000000	MN	COARSE SEA SALT
3	28	.310000	.077500	NA	COARSE SEA SALT
3	16	.000000	.000000	NI	COARSE SEA SALT
3	29	.000000	.000000	NO3	COARSE SEA SALT
3	18	.000000	.000000	PB	COARSE SEA SALT
3	30	.000000	.000000	RB	COARSE SEA SALT
3	20	.000000	.000000	SB	COARSE SEA SALT
3	31	.000000	.000000	SE	COARSE SEA SALT
3	21	.000000	.000000	SI	COARSE SEA SALT
3	22	.000000	.000000	SN	COARSE SEA SALT
3	19	.090000	.022500	SO4	COARSE SEA SALT
3	23	.000000	.000000	SR	COARSE SEA SALT
3	24	.000000	.000000	TI	COARSE SEA SALT
3	25	.000000	.000000	V	COARSE SEA SALT
3	26	.000000	.000000	ZN	COARSE SEA SALT
4	2	.002300	.000575	AL	COARSE SLASH BURN
4	3	.000000	.000000	AS	COARSE SLASH BURN
4	4	.000000	.000000	BA	COARSE SLASH BURN
4	5	.000000	.000000	BR	COARSE SLASH BURN
4	27	.523000	.130750	C	COARSE SLASH BURN
4	6	.001300	.000325	CA	COARSE SLASH BURN
4	7	.000000	.000000	CD	COARSE SLASH BURN
4	8	.009300	.002325	CL	COARSE SLASH BURN

TABLE C-4 (CONTINUED)

4	10	.000000	.000000	CR	COARSE SLASH BURN
4	11	.000000	.000000	CU	COARSE SLASH BURN
4	12	.000000	.000000	FE	COARSE SLASH BURN
4	14	.000000	.000000	K	COARSE SLASH BURN
4	15	.000090	.000022	MN	COARSE SLASH BURN
4	28	.001600	.000400	NA	COARSE SLASH BURN
4	16	.000000	.000000	NI	COARSE SLASH BURN
4	29	.010000	.002500	NO3	COARSE SLASH BURN
4	18	.000000	.000000	PB	COARSE SLASH BURN
4	30	.000000	.000000	RB	COARSE SLASH BURN
4	20	.000000	.000000	SB	COARSE SLASH BURN
4	31	.000000	.000000	SE	COARSE SLASH BURN
4	21	.054000	.013500	SI	COARSE SLASH BURN
4	22	.000000	.000000	SN	COARSE SLASH BURN
4	19	.007500	.001875	SO4	COARSE SLASH BURN
4	23	.000000	.000000	SR	COARSE SLASH BURN
4	24	.000000	.000000	TI	COARSE SLASH BURN
4	25	.000000	.000000	V	COARSE SLASH BURN
4	26	.000000	.000000	ZN	COARSE SLASH BURN
5	2	.001200	.000300	AL	COARSE AUTO W CAT
5	3	.000000	.000000	AS	COARSE AUTO W CAT
5	4	.000000	.000000	BA	COARSE AUTO W CAT
5	5	.000000	.000000	BR	COARSE AUTO W CAT
5	27	.390000	.097500	C	COARSE AUTO W CAT
5	6	.001700	.000425	CA	COARSE AUTO W CAT
5	7	.000000	.000000	CD	COARSE AUTO W CAT
5	8	.000000	.000000	CL	COARSE AUTO W CAT
5	10	.000000	.000000	CR	COARSE AUTO W CAT
5	11	.000240	.000060	CU	COARSE AUTO W CAT
5	12	.001100	.000275	FE	COARSE AUTO W CAT
5	14	.000440	.000110	K	COARSE AUTO W CAT
5	15	.000150	.000037	MN	COARSE AUTO W CAT
5	28	.000000	.000000	NA	COARSE AUTO W CAT
5	16	.000150	.000037	NI	COARSE AUTO W CAT
5	29	.000000	.000000	NO3	COARSE AUTO W CAT
5	18	.000000	.000000	PB	COARSE AUTO W CAT
5	30	.000000	.000000	RB	COARSE AUTO W CAT
5	20	.000000	.000000	SB	COARSE AUTO W CAT
5	31	.000000	.000000	SE	COARSE AUTO W CAT
5	21	.005100	.001275	SI	COARSE AUTO W CAT
5	22	.000000	.000000	SN	COARSE AUTO W CAT
5	19	.500000	.125000	SO4	COARSE AUTO W CAT
5	23	.000000	.000000	SR	COARSE AUTO W CAT
5	24	.000000	.000000	TI	COARSE AUTO W CAT
5	25	.000000	.000000	V	COARSE AUTO W CAT
5	26	.000800	.000200	ZN	COARSE AUTO W CAT

TABLE C-4 (CONTINUED)

6	2	.000430	.000108	AL	COARSE AUTO
6	3	.000000	.000000	AS	COARSE AUTO
6	4	.000000	.000000	BA	COARSE AUTO
6	5	.082000	.020500	BR	COARSE AUTO
6	27	.545000	.136250	C	COARSE AUTO
6	6	.000000	.000000	CA	COARSE AUTO
6	7	.000000	.000000	CD	COARSE AUTO
6	8	.054000	.013500	CL	COARSE AUTO
6	10	.000000	.000000	CR	COARSE AUTO
6	11	.000040	.000010	CU	COARSE AUTO
6	12	.002500	.000625	FE	COARSE AUTO
6	14	.000000	.000000	K	COARSE AUTO
6	15	.000000	.000000	MN	COARSE AUTO
6	28	.000000	.000000	NA	COARSE AUTO
6	16	.000000	.000000	NI	COARSE AUTO
6	29	.000000	.000000	NO3	COARSE AUTO
6	18	.211000	.052750	PB	COARSE AUTO
6	30	.000000	.000000	RB	COARSE AUTO
6	20	.000000	.000000	SB	COARSE AUTO
6	31	.000000	.000000	SE	COARSE AUTO
6	21	.000750	.000187	SI	COARSE AUTO
6	22	.000000	.000000	SN	COARSE AUTO
6	19	.002100	.000525	SO4	COARSE AUTO
6	23	.000000	.000000	SR	COARSE AUTO
6	24	.000000	.000000	TI	COARSE AUTO
6	25	.000000	.000000	V	COARSE AUTO
6	26	.000210	.000053	ZN	COARSE AUTO
7	2	.000000	.000000	AL	COARSE JET AIR
7	3	.000000	.000000	AS	COARSE JET AIR
7	4	.000000	.000000	BA	COARSE JET AIR
7	5	.000000	.000000	BR	COARSE JET AIR
7	27	.960000	.240000	C	COARSE JET AIR
7	6	.000000	.000000	CA	COARSE JET AIR
7	7	.000000	.000000	CD	COARSE JET AIR
7	8	.000000	.000000	CL	COARSE JET AIR
7	10	.000000	.000000	CR	COARSE JET AIR
7	11	.000000	.000000	CU	COARSE JET AIR
7	12	.000000	.000000	FE	COARSE JET AIR
7	14	.000000	.000000	K	COARSE JET AIR
7	15	.000000	.000000	MN	COARSE JET AIR
7	28	.000000	.000000	NA	COARSE JET AIR
7	16	.000000	.000000	NI	COARSE JET AIR
7	29	.000000	.000000	NO3	COARSE JET AIR
7	18	.000000	.000000	PB	COARSE JET AIR
7	30	.000000	.000000	RB	COARSE JET AIR
7	20	.000000	.000000	SB	COARSE JET AIR

TABLE C-4 (CONTINUED)

7	31	.000000	.000000	SE	COARSE JET AIR
7	21	.000000	.000000	SI	COARSE JET AIR
7	22	.000000	.000000	SN	COARSE JET AIR
7	19	.000000	.000000	SO4	COARSE JET AIR
7	23	.000000	.000000	SR	COARSE JET AIR
7	24	.000000	.000000	TI	COARSE JET AIR
7	25	.000000	.000000	V	COARSE JET AIR
7	26	.000000	.000000	ZN	COARSE JET AIR
8	2	.014700	.003675	AL	COARSE RESIDUAL OIL
8	3	.000000	.000000	AS	COARSE RESIDUAL OIL
8	4	.000000	.000000	BA	COARSE RESIDUAL OIL
8	5	.000000	.000000	BR	COARSE RESIDUAL OIL
8	27	.315000	.078750	C	COARSE RESIDUAL OIL
8	6	.035600	.008900	CA	COARSE RESIDUAL OIL
8	7	.000000	.000000	CD	COARSE RESIDUAL OIL
8	8	.007400	.001850	CL	COARSE RESIDUAL OIL
8	10	.000540	.000135	CR	COARSE RESIDUAL OIL
8	11	.000860	.000215	CU	COARSE RESIDUAL OIL
8	12	.014700	.003675	FE	COARSE RESIDUAL OIL
8	14	.000000	.000000	K	COARSE RESIDUAL OIL
8	15	.000270	.000068	MN	COARSE RESIDUAL OIL
8	28	.009000	.002250	NA	COARSE RESIDUAL OIL
8	16	.013900	.003475	NI	COARSE RESIDUAL OIL
8	29	.000000	.000000	NO3	COARSE RESIDUAL OIL
8	18	.000000	.000000	PB	COARSE RESIDUAL OIL
8	30	.000000	.000000	RB	COARSE RESIDUAL OIL
8	20	.000000	.000000	SB	COARSE RESIDUAL OIL
8	31	.000000	.000000	SE	COARSE RESIDUAL OIL
8	21	.037000	.009250	SI	COARSE RESIDUAL OIL
8	22	.000000	.000000	SN	COARSE RESIDUAL OIL
8	19	.073000	.018250	SO4	COARSE RESIDUAL OIL
8	23	.000000	.000000	SR	COARSE RESIDUAL OIL
8	24	.001400	.000350	TI	COARSE RESIDUAL OIL
8	25	.017900	.004475	V	COARSE RESIDUAL OIL
8	26	.000500	.000125	ZN	COARSE RESIDUAL OIL
9	2	.005900	.001475	AL	COARSE DISTILLATE OIL
9	3	.000000	.000000	AS	COARSE DISTILLATE OIL
9	4	.000000	.000000	BA	COARSE DISTILLATE OIL
9	5	.000000	.000000	BR	COARSE DISTILLATE OIL
9	27	.172000	.043000	C	COARSE DISTILLATE OIL
9	6	.005000	.001250	CA	COARSE DISTILLATE OIL
9	7	.000000	.000000	CD	COARSE DISTILLATE OIL
9	8	.016000	.004000	CL	COARSE DISTILLATE OIL
9	10	.000000	.000000	CR	COARSE DISTILLATE OIL
9	11	.001100	.000275	CU	COARSE DISTILLATE OIL
9	12	.002300	.000575	FE	COARSE DISTILLATE OIL

TABLE C-4 (CONTINUED)

9	14	.000000	.000000	K	COARSE DISTILLATE OIL
9	15	.000130	.000033	MN	COARSE DISTILLATE OIL
9	28	.006900	.001725	NA	COARSE DISTILLATE OIL
9	16	.000000	.000000	NI	COARSE DISTILLATE OIL
9	29	.000000	.000000	NO3	COARSE DISTILLATE OIL
9	18	.000000	.000000	PB	COARSE DISTILLATE OIL
9	30	.000000	.000000	RB	COARSE DISTILLATE OIL
9	20	.000000	.000000	SB	COARSE DISTILLATE OIL
9	31	.000000	.000000	SE	COARSE DISTILLATE OIL
9	21	.002900	.000725	SI	COARSE DISTILLATE OIL
9	22	.000000	.000000	SN	COARSE DISTILLATE OIL
9	19	.000000	.000000	SO4	COARSE DISTILLATE OIL
9	23	.000000	.000000	SR	COARSE DISTILLATE OIL
9	24	.000000	.000000	TI	COARSE DISTILLATE OIL
9	25	.000000	.000000	V	COARSE DISTILLATE OIL
9	26	.000000	.000000	ZN	COARSE DISTILLATE OIL
10	2	.000000	.000000	AL	COARSE RESIDENTIAL GAS
10	3	.000000	.000000	AS	COARSE RESIDENTIAL GAS
10	4	.000000	.000000	BA	COARSE RESIDENTIAL GAS
10	5	.000000	.000000	BR	COARSE RESIDENTIAL GAS
10	27	.120000	.030000	C	COARSE RESIDENTIAL GAS
10	6	.050000	.012500	CA	COARSE RESIDENTIAL GAS
10	7	.000000	.000000	CD	COARSE RESIDENTIAL GAS
10	8	.000000	.000000	CL	COARSE RESIDENTIAL GAS
10	10	.000000	.000000	CR	COARSE RESIDENTIAL GAS
10	11	.000000	.000000	CU	COARSE RESIDENTIAL GAS
10	12	.000000	.000000	FE	COARSE RESIDENTIAL GAS
10	14	.000000	.000000	K	COARSE RESIDENTIAL GAS
10	15	.000000	.000000	MN	COARSE RESIDENTIAL GAS
10	28	.000000	.000000	NA	COARSE RESIDENTIAL GAS
10	16	.000000	.000000	NI	COARSE RESIDENTIAL GAS
10	29	.000000	.000000	NO3	COARSE RESIDENTIAL GAS
10	18	.000000	.000000	PB	COARSE RESIDENTIAL GAS
10	30	.000000	.000000	RB	COARSE RESIDENTIAL GAS
10	20	.000000	.000000	SB	COARSE RESIDENTIAL GAS
10	31	.000000	.000000	SE	COARSE RESIDENTIAL GAS
10	21	.000000	.000000	SI	COARSE RESIDENTIAL GAS
10	22	.000000	.000000	SN	COARSE RESIDENTIAL GAS
10	19	.470000	.117500	SO4	COARSE RESIDENTIAL GAS
10	23	.000000	.000000	SR	COARSE RESIDENTIAL GAS
10	24	.000000	.000000	TI	COARSE RESIDENTIAL GAS
10	25	.000000	.000000	V	COARSE RESIDENTIAL GAS
10	26	.000000	.000000	ZN	COARSE RESIDENTIAL GAS

TABLE C-4 (CONTINUED)

11	2	.000000	.000000	AL	COARSE COAL
11	3	.000000	.000000	AS	COARSE COAL
11	4	.000000	.000000	BA	COARSE COAL
11	5	.000000	.000000	BR	COARSE COAL
11	27	.000000	.000000	C	COARSE COAL
11	6	.023600	.005900	CA	COARSE COAL
11	7	.000000	.000000	CD	COARSE COAL
11	8	.000000	.000000	CL	COARSE COAL
11	10	.000000	.000000	CR	COARSE COAL
11	11	.000000	.000000	CU	COARSE COAL
11	12	.040990	.010248	FE	COARSE COAL
11	14	.000000	.000000	K	COARSE COAL
11	15	.000000	.000000	MN	COARSE COAL
11	28	.000000	.000000	NA	COARSE COAL
11	16	.000000	.000000	NI	COARSE COAL
11	29	.000000	.000000	NO3	COARSE COAL
11	18	.000000	.000000	PB	COARSE COAL
11	30	.000000	.000000	RB	COARSE COAL
11	20	.000000	.000000	SB	COARSE COAL
11	31	.000000	.000000	SE	COARSE COAL
11	21	.032920	.008230	SI	COARSE COAL
11	22	.000000	.000000	SN	COARSE COAL
11	19	.121120	.030280	SO4	COARSE COAL
11	23	.000000	.000000	SR	COARSE COAL
11	24	.000000	.000000	TI	COARSE COAL
11	25	.000000	.000000	V	COARSE COAL
11	26	.006830	.001708	ZN	COARSE COAL
12	2	.002800	.000700	AL	COARSE KRAFT REC BOILER
12	3	.000000	.000000	AS	COARSE KRAFT REC BOILER
12	4	.000000	.000000	BA	COARSE KRAFT REC BOILER
12	5	.000560	.000140	BR	COARSE KRAFT REC BOILER
12	27	.176000	.044000	C	COARSE KRAFT REC BOILER
12	6	.003600	.000900	CA	COARSE KRAFT REC BOILER
12	7	.000000	.000000	CD	COARSE KRAFT REC BOILER
12	8	.029000	.007250	CL	COARSE KRAFT REC BOILER
12	10	.004800	.001200	CR	COARSE KRAFT REC BOILER
12	11	.000600	.000150	CU	COARSE KRAFT REC BOILER
12	12	.018400	.004600	FE	COARSE KRAFT REC BOILER
12	14	.004000	.001000	K	COARSE KRAFT REC BOILER
12	15	.000520	.000130	MN	COARSE KRAFT REC BOILER
12	28	.053000	.013250	NA	COARSE KRAFT REC BOILER
12	16	.002200	.000550	NI	COARSE KRAFT REC BOILER
12	29	.000000	.000000	NO3	COARSE KRAFT REC BOILER
12	18	.000000	.000000	PB	COARSE KRAFT REC BOILER

TABLE C-4 (CONTINUED)

12	30	.000000	.000000	RB	COARSE KRAFT REC BOILER
12	20	.000000	.000000	SB	COARSE KRAFT REC BOILER
12	31	.000000	.000000	SE	COARSE KRAFT REC BOILER
12	21	.001300	.000325	SI	COARSE KRAFT REC BOILER
12	22	.000000	.000000	SN	COARSE KRAFT REC BOILER
12	19	.118000	.029500	SO4	COARSE KRAFT REC BOILER
12	23	.000000	.000000	SR	COARSE KRAFT REC BOILER
12	24	.000000	.000000	TI	COARSE KRAFT REC BOILER
12	25	.000000	.000000	V	COARSE KRAFT REC BOILER
12	26	.000000	.000000	ZN	COARSE KRAFT REC BOILER
13	2	.000000	.000000	AL	COARSE ELEC ARC FURN
13	3	.000000	.000000	AS	COARSE ELEC ARC FURN
13	4	.000000	.000000	BA	COARSE ELEC ARC FURN
13	5	.000000	.000000	BR	COARSE ELEC ARC FURN
13	27	.000000	.000000	C	COARSE ELEC ARC FURN
13	6	.069000	.017250	CA	COARSE ELEC ARC FURN
13	7	.000000	.000000	CD	COARSE ELEC ARC FURN
13	8	.038000	.009500	CL	COARSE ELEC ARC FURN
13	10	.021000	.005250	CR	COARSE ELEC ARC FURN
13	11	.004300	.001075	CU	COARSE ELEC ARC FURN
13	12	.308000	.077000	FE	COARSE ELEC ARC FURN
13	14	.005600	.001400	K	COARSE ELEC ARC FURN
13	15	.095000	.023750	MN	COARSE ELEC ARC FURN
13	28	.014000	.003500	NA	COARSE ELEC ARC FURN
13	16	.006200	.001550	NI	COARSE ELEC ARC FURN
13	29	.000000	.000000	NO3	COARSE ELEC ARC FURN
13	18	.006400	.001600	PB	COARSE ELEC ARC FURN
13	30	.000000	.000000	RB	COARSE ELEC ARC FURN
13	20	.000000	.000000	SB	COARSE ELEC ARC FURN
13	31	.000000	.000000	SE	COARSE ELEC ARC FURN
13	21	.066000	.016500	SI	COARSE ELEC ARC FURN
13	22	.000000	.000000	SN	COARSE ELEC ARC FURN
13	19	.013000	.003250	SO4	COARSE ELEC ARC FURN
13	23	.000000	.000000	SR	COARSE ELEC ARC FURN
13	24	.001100	.000275	TI	COARSE ELEC ARC FURN
13	25	.000580	.000145	V	COARSE ELEC ARC FURN
13	26	.012000	.003000	ZN	COARSE ELEC ARC FURN
14	2	.001800	.000450	AL	COARSE FERROMANGANESE FURN
14	3	.000000	.000000	AS	COARSE FERROMANGANESE FURN
14	4	.000000	.000000	BA	COARSE FERROMANGANESE FURN
14	5	.000000	.000000	BR	COARSE FERROMANGANESE FURN
14	27	.190000	.047500	C	COARSE FERROMANGANESE FURN
14	6	.005700	.001425	CA	COARSE FERROMANGANESE FURN
14	7	.000000	.000000	CD	COARSE FERROMANGANESE FURN
14	8	.008500	.002125	CL	COARSE FERROMANGANESE FURN
14	10	.000230	.000057	CR	COARSE FERROMANGANESE FURN
14	11	.000740	.000185	CU	COARSE FERROMANGANESE FURN

TABLE C-4 (CONTINUED)

14	12	.003800	.000950	FE	COARSE FERROMANGANESE FURN
14	14	.012000	.003000	K	COARSE FERROMANGANESE FURN
14	15	.027500	.006875	MN	COARSE FERROMANGANESE FURN
14	28	.003400	.000850	NA	COARSE FERROMANGANESE FURN
14	16	.000000	.000000	NI	COARSE FERROMANGANESE FURN
14	29	.012000	.003000	NO3	COARSE FERROMANGANESE FURN
14	18	.000000	.000000	PB	COARSE FERROMANGANESE FURN
14	30	.000000	.000000	RB	COARSE FERROMANGANESE FURN
14	20	.000000	.000000	SB	COARSE FERROMANGANESE FURN
14	31	.000000	.000000	SE	COARSE FERROMANGANESE FURN
14	21	.002900	.000725	SI	COARSE FERROMANGANESE FURN
14	22	.000000	.000000	SN	COARSE FERROMANGANESE FURN
14	19	.011000	.002750	SO4	COARSE FERROMANGANESE FURN
14	23	.000000	.000000	SR	COARSE FERROMANGANESE FURN
14	24	.000000	.000000	TI	COARSE FERROMANGANESE FURN
14	25	.000090	.000022	V	COARSE FERROMANGANESE FURN
14	26	.000350	.000087	ZN	COARSE FERROMANGANESE FURN
15	2	.000000	.000000	AL	COARSE CALCINATION OF GYPSUM
15	3	.000000	.000000	AS	COARSE CALCINATION OF GYPSUM
15	4	.000000	.000000	BA	COARSE CALCINATION OF GYPSUM
15	5	.000000	.000000	BR	COARSE CALCINATION OF GYPSUM
15	27	.000000	.000000	C	COARSE CALCINATION OF GYPSUM
15	6	.090000	.022500	CA	COARSE CALCINATION OF GYPSUM
15	7	.000000	.000000	CD	COARSE CALCINATION OF GYPSUM
15	8	.000000	.000000	CL	COARSE CALCINATION OF GYPSUM
15	10	.000000	.000000	CR	COARSE CALCINATION OF GYPSUM
15	11	.000000	.000000	CU	COARSE CALCINATION OF GYPSUM
15	12	.000000	.000000	FE	COARSE CALCINATION OF GYPSUM
15	14	.000000	.000000	K	COARSE CALCINATION OF GYPSUM
15	15	.000000	.000000	MN	COARSE CALCINATION OF GYPSUM
15	28	.000000	.000000	NA	COARSE CALCINATION OF GYPSUM
15	16	.000000	.000000	NI	COARSE CALCINATION OF GYPSUM
15	29	.000000	.000000	NO3	COARSE CALCINATION OF GYPSUM
15	18	.000000	.000000	PB	COARSE CALCINATION OF GYPSUM
15	30	.000000	.000000	RB	COARSE CALCINATION OF GYPSUM
15	20	.000000	.000000	SB	COARSE CALCINATION OF GYPSUM
15	31	.000000	.000000	SE	COARSE CALCINATION OF GYPSUM
15	21	.000000	.000000	SI	COARSE CALCINATION OF GYPSUM
15	22	.000000	.000000	SN	COARSE CALCINATION OF GYPSUM
15	19	.570000	.142500	SO4	COARSE CALCINATION OF GYPSUM
15	23	.000000	.000000	SR	COARSE CALCINATION OF GYPSUM
15	24	.000000	.000000	TI	COARSE CALCINATION OF GYPSUM
15	25	.000000	.000000	V	COARSE CALCINATION OF GYPSUM
15	26	.000000	.000000	ZN	COARSE CALCINATION OF GYPSUM
16	2	.000000	.000000	AL	COARSE CEMENT
16	3	.000000	.000000	AS	COARSE CEMENT

TABLE C-4 (CONTINUED)

16	4	.000000	.000000	BA	COARSE CEMENT
16	5	.000000	.000000	BR	COARSE CEMENT
16	27	.190000	.047500	C	COARSE CEMENT
16	6	.200000	.050000	CA	COARSE CEMENT
16	7	.000000	.000000	CD	COARSE CEMENT
16	8	.000000	.000000	CL	COARSE CEMENT
16	10	.000000	.000000	CR	COARSE CEMENT
16	11	.000000	.000000	CU	COARSE CEMENT
16	12	.000000	.000000	FE	COARSE CEMENT
16	14	.020000	.005000	K	COARSE CEMENT
16	15	.000000	.000000	MN	COARSE CEMENT
16	28	.000000	.000000	NA	COARSE CEMENT
16	16	.000000	.000000	NI	COARSE CEMENT
16	29	.000000	.000000	NO3	COARSE CEMENT
16	18	.000000	.000000	PB	COARSE CEMENT
16	30	.000000	.000000	RB	COARSE CEMENT
16	20	.000000	.000000	SB	COARSE CEMENT
16	31	.000000	.000000	SE	COARSE CEMENT
16	21	.100000	.025000	SI	COARSE CEMENT
16	22	.000000	.000000	SN	COARSE CEMENT
16	19	.030000	.007500	SO4	COARSE CEMENT
16	23	.000000	.000000	SR	COARSE CEMENT
16	24	.000000	.000000	TI	COARSE CEMENT
16	25	.000000	.000000	V	COARSE CEMENT
16	26	.000000	.000000	ZN	COARSE CEMENT
17	2	.000000	.000000	AL	PETROL-FCC UNDTs
17	3	.000000	.000000	AS	PETROL-FCC UNDTs
17	4	.000000	.000000	BA	PETROL-FCC UNDTs
17	5	.000000	.000000	BR	PETROL-FCC UNDTs
17	27	.000000	.000000	C	PETROL-FCC UNDTs
17	6	.000000	.000000	CA	PETROL-FCC UNDTs
17	7	.000000	.000000	CD	PETROL-FCC UNDTs
17	8	.000000	.000000	CL	PETROL-FCC UNDTs
17	10	.000000	.000000	CR	PETROL-FCC UNDTs
17	11	.000000	.000000	CU	PETROL-FCC UNDTs
17	12	.005000	.001250	FE	PETROL-FCC UNDTs
17	14	.000000	.000000	K	PETROL-FCC UNDTs
17	15	.000000	.000000	MN	PETROL-FCC UNDTs
17	28	.000000	.000000	NA	PETROL-FCC UNDTs
17	16	.000000	.000000	NI	PETROL-FCC UNDTs
17	29	.000000	.000000	NO3	PETROL-FCC UNDTs
17	18	.000000	.000000	PB	PETROL-FCC UNDTs
17	30	.000000	.000000	RB	PETROL-FCC UNDTs
17	20	.000000	.000000	SB	PETROL-FCC UNDTs
17	31	.000000	.000000	SE	PETROL-FCC UNDTs
17	21	.200000	.050000	SI	PETROL-FCC UNDTs

TABLE C-4 (CONTINUED)

17	22	.000000	.000000	SN	PETROL-FCC UNDTs
17	19	.070000	.017500	SO4	PETROL-FCC UNDTs
17	23	.000000	.000000	SR	PETROL-FCC UNDTs
17	24	.000000	.000000	TI	PETROL-FCC UNDTs
17	25	.000000	.000000	V	PETROL-FCC UNDTs
17	26	.000000	.000000	ZN	PETROL-FCC UNDTs
18	2	.000000	.000000	AL	COARSE LS KILN
18	3	.000000	.000000	AS	COARSE LS KILN
18	4	.000000	.000000	BA	COARSE LS KILN
18	5	.000000	.000000	BR	COARSE LS KILN
18	27	.400000	.100000	C	COARSE LS KILN
18	6	.300000	.075000	CA	COARSE LS KILN
18	7	.000000	.000000	CD	COARSE LS KILN
18	8	.000000	.000000	CL	COARSE LS KILN
18	10	.000000	.000000	CR	COARSE LS KILN
18	11	.000000	.000000	CU	COARSE LS KILN
18	12	.020000	.005000	FE	COARSE LS KILN
18	14	.000000	.000000	K	COARSE LS KILN
18	15	.000000	.000000	MN	COARSE LS KILN
18	28	.000000	.000000	NA	COARSE LS KILN
18	16	.000000	.000000	NI	COARSE LS KILN
18	29	.000000	.000000	NO3	COARSE LS KILN
18	18	.000000	.000000	PB	COARSE LS KILN
18	30	.000000	.000000	RB	COARSE LS KILN
18	20	.000000	.000000	SB	COARSE LS KILN
18	31	.100000	.025000	SE	COARSE LS KILN
18	21	.000000	.000000	SI	COARSE LS KILN
18	22	.000000	.000000	SN	COARSE LS KILN
18	19	.000000	.000000	SO4	COARSE LS KILN
18	23	.000000	.000000	SR	COARSE LS KILN
18	24	.000000	.000000	TI	COARSE LS KILN
18	25	.000000	.000000	V	COARSE LS KILN
18	26	.000000	.000000	ZN	COARSE LS KILN
19	2	.000000	.000000	AL	COARSE SECONDARY SO4
19	3	.000000	.000000	AS	COARSE SECONDARY SO4
19	4	.000000	.000000	BA	COARSE SECONDARY SO4
19	5	.000000	.000000	BR	COARSE SECONDARY SO4
19	27	.000000	.000000	C	COARSE SECONDARY SO4
19	6	.000000	.000000	CA	COARSE SECONDARY SO4
19	7	.000000	.000000	CD	COARSE SECONDARY SO4
19	8	.000000	.000000	CL	COARSE SECONDARY SO4
19	10	.000000	.000000	CR	COARSE SECONDARY SO4
19	11	.000000	.000000	CU	COARSE SECONDARY SO4
19	12	.000000	.000000	FE	COARSE SECONDARY SO4
19	14	.000000	.000000	K	COARSE SECONDARY SO4
19	15	.000000	.000000	MN	COARSE SECONDARY SO4
19	28	.000000	.000000	NA	COARSE SECONDARY SO4

TABLE C-4 (CONTINUED)

19	16	.000000	.000000	NI	COARSE SECONDARY SO4
19	29	.000000	.000000	NO3	COARSE SECONDARY SO4
19	18	.000000	.000000	PB	COARSE SECONDARY SO4
19	30	.000000	.000000	RB	COARSE SECONDARY SO4
19	20	.000000	.000000	SB	COARSE SECONDARY SO4
19	31	.000000	.000000	SE	COARSE SECONDARY SO4
19	21	.000000	.000000	SI	COARSE SECONDARY SO4
19	22	.000000	.000000	SN	COARSE SECONDARY SO4
19	19	1.000000	.000000	SO4	COARSE SECONDARY SO4
19	23	.000000	.000000	SR	COARSE SECONDARY SO4
19	24	.000000	.000000	TI	COARSE SECONDARY SO4
19	25	.000000	.000000	V	COARSE SECONDARY SO4
19	26	.000000	.000000	ZN	COARSE SECONDARY SO4

TABLE C-5. RECEPTOR CONCENTRATION INPUT FILE

03 URBAN CORE	810229 12 07	12				
30		1	35.	7.	75.	7.
30		2	.088	.062	1.951	.422
30		3	.036	.007	.004	.004
30		4	.149	.014	.371	.023
30		5	.344	.017	.108	.007
30		6	.441	.023	13.014	1.442
30		7	.004	.002	.0005	.001
30		8	.051	.007	.288	.068
30		9	.003	.002	.015	.003
30		10	.002	.004	.022	.005
30		11	.013	.002	.018	.002
30		12	.208	.011	1.871	.118
30		13	0.	.003	.001	.002
30		14	.165	.009	.517	.072
30		15	.022	.004	.088	.008
30		16	.006	.001	.003	.001
30		17	.119	.017	.102	.040
30		18	1.422	.068	.346	.024
30		19	13.13	.681	1.725	.939
30		20	.003	.002	.004	.002
30		21	.277	.031	8.652	1.987
30		22	.001	.002	.005	.002
30		23	.003	.001	.030	.003
30		24	.007	.014	.205	.037
30		25	.002	.008	.007	.014
30		26	.042	.003	.071	.006
03 BACKGROUND	810229 12 07	12				
30		1	28.	3.	37.	4.
30		2	.070	.055	.739	.171
30		3	.014	.006	.001	.004
30		4	.146	.018	.086	.016
30		5	.164	.010	.064	.005
30		6	.128	.008	3.805	.444
30		7	.001	.002	.001	.002
30		8	.010	.007	.014	.010
30		9	.008	.003	.001	.003
30		10	.010	.005	.0025	.005
30		11	.027	.003	.004	.002
30		12	.120	.008	.692	.044
30		13	.0015	.003	.009	.003
30		14	.186	.010	.215	.032
30		15	.022	.004	.018	.004
30		16	.003	.002	.001	.002

TABLE C-5 (CONTINUED)

30	17	.103	.018	.020	.022
30	18	.894	.047	.213	.017
30	19	14.78	.765	.852	.783
30	20	.008	.003	.001	.003
30	21	.189	.027	4.0	.914
30	22	.024	.003	.003	.003
30	23	.003	.002	.006	.002
30	24	.008	.016	.097	.017
30	25	.003	.009	.0035	.007
30	26	.038	.003	.016	.003

TABLE C-6. SUMMARY HARDCOPY OUTPUT FILE

*** CMB SOURCE CONTRIBUTION SUMMARY ***

RESULTS FOR CMB SITE: URBAN CORE YEAR: 81 DATE: 0229
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO

SOURCE	FINE			COARSE			TOTAL		
	UG/M3	Σ	UG/M3	UG/M3	Σ	UG/M3	UG/M3	Σ	UG/M3
INTERCEPT	.004 +- .004		.011 +- .005			.015 +- .006			
SOIL	-.509 +- 3.092	4.419 +- 8.838	36.445 +- 18.752	48.593 +- 25.410	35.936 +- 19.005	32.669 +- 17.525			
RD DUST	-.024 +- .923	1.318 +- 2.636	13.578 +- 6.185	18.104 +- 8.418	13.554 +- 6.254	12.321 +- 5.792			
SEA SALT	-.446 +- .171	.276 +- .552	.177 +- .491	.328 +- .655	-.270 +- .520	.237 +- .473			
AUTO CAT	7.377 +- 20.436	29.271 +- 58.541	10.339 +- 13.655	9.126 +- 18.252	17.717 +- 24.579	11.196 +- 22.391			
AUTO	4.635 +- .941	13.244 +- 3.773	.722 +- .275	.963 +- .378	5.358 +- .980	4.871 +- .993			
DIST OIL	3.596 +- 6.614	9.505 +- 19.009	.000 +- .000	.000 +- .000	3.596 +- 6.614	3.010 +- 6.020			
RES GAS	1.015 +- 5.311	7.593 +- 15.186	.000 +- .000	.000 +- .000	1.015 +- 5.311	2.415 +- 4.829			
COAL	1.771 +- 1.348	5.059 +- 3.981	4.532 +- 3.137	6.043 +- 4.220	6.303 +- 3.414	5.730 +- 3.146			
KRAFT RB	.000 +- .000	.000 +- .000	2.229 +- 3.455	2.308 +- 4.615	2.229 +- 3.455	1.573 +- 3.146			
ELARCFM	.076 +- .454	.648 +- 1.296	.000 +- .000	.000 +- .000	.076 +- .454	.206 +- .412			
FERRMFR	.061 +- .250	.358 +- .715	.000 +- .000	.000 +- .000	.061 +- .250	.114 +- .227			
CEMENT	7.403 +- 2.919	21.151 +- 9.353	13.874 +- 11.324	18.499 +- 15.197	21.277 +- 11.694	19.343 +- 10.773			
PET FCC	8.221 +- 12.252	17.660 +- 35.320	.000 +- .000	.000 +- .000	8.221 +- 12.252	5.579 +- 11.159			
SEC S04	-.187 +- 11.012	15.732 +- 31.464	.000 +- .000	.000 +- .000	-.187 +- 11.012	5.006 +- 10.011			
CALC.MASS	32.991 +- 15.162	94.261 +- 47.244	81.908 +- 25.267	109.210 +- 35.197	114.899 +- 29.467	104.454 +- .001			
MEAS.MASS	35.000 +- 7.000		75.000 +- 7.000		110.000 +- 9.899				

TABLE C-6 (CONTINUED)

*** CMB SOURCE CONTRIBUTION SUMMARY ***

RESULTS FOR CMB SITE: BACKGROUND YEAR: 81 DATE: 0229
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO

SOURCE	FINE			COARSE			TOTAL		
	UG/M3	Z	Z	UG/M3	Z	Z	UG/M3	Z	Z
INTERCEPT	.006 +- .006			.003 +- .002			.009 +- .006		
SOIL	-.334 +- .346	.622 +- 1.243	54.738 +- 16.911	5.861			19.919 +- 5.872	30.645 +- 9.336	
RD DUST	.214 +- .656	1.171 +- 2.343	16.567 +- 4.097	1.363			6.343 +- 1.513	9.759 +- 2.445	
SEA SALT	-.187 +- .093	.170 +- .341	.042 +- .084	.031			-.211 +- .098	.077 +- .153	
AUTO CAT	12.538 +- 7.325	44.778 +- 26.596	1.749 +- 4.822	4.822			14.287 +- 8.770	21.980 +- 13.597	
AUTO	1.889 +- .609	6.745 +- 2.291	1.460 +- .327	.106			2.429 +- .618	3.736 +- .993	
DIST OIL	1.572 +- 3.786	6.768 +- 13.536	.000 +- .000	.000			1.572 +- 3.786	2.914 +- 5.828	
RES GAS	-.735 +- .733	1.316 +- 2.632	.000 +- .000	.000			-.735 +- .733	.565 +- 1.131	
COAL	1.088 +- .951	3.887 +- 3.420	1.397 +- .840	.840			2.485 +- 1.269	3.823 +- 1.974	
KRAFT RB	.000 +- .000	.000 +- .000	.726 +- 1.453	.538			.053 +- .538	.413 +- .827	
ELARCFM	-.053 +- .114	.204 +- .408	.000 +- .000	.000			-.053 +- .114	.088 +- .176	
FERRMFR	.147 +- .137	.523 +- .492	.000 +- .000	.000			.147 +- .137	.225 +- .211	
CEMENT	2.884 +- 1.166	10.300 +- 4.307	18.796 +- 7.558	2.694			9.838 +- 2.935	15.136 +- 4.663	
PET FCC	4.596 +- 4.504	16.416 +- 16.183	.000 +- .000	.000			4.596 +- 4.504	7.071 +- 6.951	
SEC S04	4.025 +- 4.481	8.038 +- 16.076	.000 +- .000	.000			4.025 +- 4.481	3.455 +- 6.910	
CALC.MASS	27.650 +- 7.882	98.750 +- 30.073	37.055 +- 13.502	100.148 +- 38.064			64.705 +- 15.634	99.546 +- .002	
MEAS.MASS	28.000 +- 3.000		37.000 +- 4.000				65.000 +- 5.000		

TABLE C-7. GENERAL HARDCOPY OUTPUT FILE

RESULTS FOR CMB SITE: URBAN CORE YEAR: 81 DATE: 0229
 COARSE PARTICULATE FRACTION
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO

		RIDGE REGRESSION				LEAST SQUARES			
		K= .800		R-SQUARE: .6151		K=0.0		R-SQUARE: .7702	
CODE	SOURCE	UG/M3		Z		UG/M3		VIF	
	INTERCEPT	.011+-	.005			.023+-	.010		
1	SOIL	36.445+-	18.752	48.593+-	25.410	77.894+-	81.347	6.178	
2	RD DUST	13.578+-	6.185	18.104+-	8.418	18.281+-	13.310	2.184	
3	SEA SALT	.177+-	.491	.328+-	.655	.365+-	.771	1.223	
5	AUTO CAT	10.339+-	13.655	9.126+-	18.252	-51.096+-	63.596	6.754	
6	AUTO	.722+-	.275	.963+-	.378	1.180+-	.395	1.054	
9	DIST OIL	.000+-	.000	.000+-	.000	.000+-	.000	.000	
10	RES GAS	.000+-	.000	.000+-	.000	.000+-	.000	.000	
11	COAL	4.532+-	3.137	6.043+-	4.220	11.906+-	7.909	2.829	
12	KRAFT RB	2.229+-	3.455	2.308+-	4.615	-.031+-	6.302	1.564	
13	ELARCFRN	.000+-	.000	.000+-	.000	.000+-	.000	.000	
14	FERRMNFR	.000+-	.000	.000+-	.000	.000+-	.000	.000	
16	CEMENT	13.874+-	11.324	18.499+-	15.197	23.364+-	20.317	1.550	
17	PET FCC	.000+-	.000	.000+-	.000	.000+-	.000	.000	
19	SEC S04	.000+-	.000	.000+-	.000	.000+-	.000	.000	
TOTAL:		81.908+-	25.267	109.210+-	35.197	81.884+-	43.046		

SPECIES CODE	FIT FLG	MISS FLG	COARSE MEAS. UG/M3	SUSPENDED PERCENT	PARTICULATE CALC. UG/M3	RATIO					
1	TOTAL	*	75.000+-	7.000	100.000+-13.199	81.908+-25.267	1.092+-	.499	TOTAL		
2	AL	*	1.951+-	.422	2.601+-	.613	1.125+-	.229	.577+-	.136	AL
3	AS		.004+-	.004	.003+-	.005	.011+-	.000	2.762+-	.000	AS
4	BA	*	.371+-	.023	.495+-	.055	.011+-	.000	.030+-	.000	BA
5	BR	*	.108+-	.007	.144+-	.016	.073+-	.015	.672+-	.165	BR
6	CA	*	13.014+-	1.442	17.352+-	2.514	5.186+-	.842	.399+-	.070	CA
7	CD		<	.001	<	.001	.011+-	.000	22.097+-	.000	CD
8	CL	*	.288+-	.068	.384+-	.097	.212+-	.031	.736+-	.133	CL
9	CO	*	.015+-	.003	.020+-	.004	.011+-	.000	.737+-	.035	CO
10	CR	*	.022+-	.005	.029+-	.007	.022+-	.003	.989+-	.171	CR
11	CU	*	.018+-	.002	.024+-	.003	.018+-	.001	1.010+-	.084	CU
12	FE	*	1.871+-	.118	2.495+-	.281	1.204+-	.205	.643+-	.130	FE
13	HG		<	.001	<	.003	.011+-	.000	11.048+-	4.756	HG
14	K	*	.517+-	.072	.689+-	.116	.347+-	.070	.672+-	.164	K
15	MN	*	.088+-	.008	.117+-	.015	.035+-	.004	.398+-	.048	MN
16	NI		.003+-	.001	.004+-	.001	.018+-	.001	5.834+-	2.534	NI
17	P	*	.102+-	.040	.136+-	.055	.011+-	.000	.108+-	.004	P
18	PB	*	.346+-	.024	.461+-	.054	.171+-	.038	.494+-	.123	PB
19	S04		1.725+-	.939	2.300+-	1.270	6.525+-	1.306	3.782+-	2.962	S04
20	SB		.004+-	.002	.005+-	.003	.011+-	.000	2.762+-	.000	SB
21	SI	*	8.652+-	1.987	11.536+-	2.860	6.335+-	1.048	.732+-	.150	SI
22	SN		.005+-	.002	.007+-	.003	.011+-	.000	2.210+-	.000	SN
23	SR	*	.030+-	.003	.040+-	.005	.016+-	.001	.538+-	.048	SR
24	TI	*	.205+-	.037	.273+-	.056	.181+-	.035	.881+-	.229	TI
25	V		<	.007	<	.019	.015+-	.001	2.102+-	.307	V
26	ZN	*	.071+-	.006	.095+-	.012	.054+-	.008	.756+-	.142	ZN
27	C	M	<	.000	<	.001	8.129+-	1.224	.000+-	.000	C
28	NA	M	<	.000	<	.001	.422+-	.068	.000+-	.000	NA
29	NO3	M	<	.000	<	.001	.014+-	.001	.000+-	.000	NO3
30	RB	M	<	.000	<	.001	.012+-	.000	.000+-	.000	RB
31	SE	M	<	.000	<	.001	.011+-	.000	.000+-	.000	SE

MEASURED AMBIENT MASS (UG/M3): FINE: 35.0+- 7.0 COARSE: 75.0+- 7.0 TOTAL: 110.0+- 9.9

TABLE C-7 (CONTINUED)

RESULTS FOR CMB SITE: URBAN CORE YEAR: 81 DATE: 0229

FINE PARTICULATE FRACTION

SAMPLING DURATION: 12 HRS. WITH START HOUR: 7

BACKGROUND SITE SUBTRACTED: NO

RIDGE REGRESSION

K= .010 R-SQUARE: .9179

LEAST SQUARES

K=0.0 R-SQUARE: .9200

CODE	SOURCE	UG/M3	%	UG/M3	VIF
	INTERCEPT	.004+- .004		.005+- .006	
1	SOIL	-.509+- .923	4.419+- 8.838	-8.858+- 27.313	432.869
2	RD DUST	-.024+- .923	1.318+- 2.636	.891+- 3.239	29.638
3	SEA SALT	-.446+- .171	.276+- .552	-.533+- .265	14.234
5	AUTO CAT	7.377+- 20.436	29.271+- 58.541	-2.525+- 58.257	79.398
6	AUTO	4.635+- .941	13.244+- 3.773	4.800+- .975	2.881
9	DIST OIL	3.596+- 6.614	9.505+- 19.009	6.549+- 10.723	14.366
10	RES GAS	1.015+- 5.311	7.593+- 15.186	15.427+- 49.140	413.108
11	COAL	1.771+- 1.348	5.059+- 3.981	2.192+- 2.462	9.374
13	ELARCFRN	.076+- .454	.648+- 1.296	.048+- 1.249	71.640
14	FERRMFR	.061+- .250	.358+- .715	.083+- .612	24.698
16	CEMENT	7.403+- 2.919	21.151+- 9.353	7.999+- 4.322	6.798
17	PET FCC	8.221+- 12.252	17.660+- 35.320	9.410+- 41.216	77.121
19	SEC SO4	-.187+- 11.012	15.732+- 31.464	-3.353+- 49.346	173.618
TOTAL:		32.991+- 15.162	94.261+- 47.244	32.136+- 50.953	

SPECIES CODE	FIT FLG	MISS FLG	FINE MEAS. UG/M3	SUSPENDED PARTICULATE PERCENT	CALC. UG/M3	RATIO
1	TOTAL	*	35.000+- 7.000	100.000+- 28.284	32.991+- 15.162	.943+- .595 TOTAL
2	AL	*	.088+- .062	.251+- .184	.029+- .004	.331+- .050 AL
3	AS	*	.036+- .007	.103+- .029	.004+- .000	.109+- .000 AS
4	BA	*	.149+- .014	.426+- .094	.004+- .000	.028+- .000 BA
5	BR	*	.344+- .017	.983+- .202	.385+- .095	1.119+- .415 BR
6	CA	*	.441+- .023	1.260+- .260	.441+- .095	.999+- .303 CA
7	CD	*	.004+- .002	.011+- .006	.006+- .000	1.375+- .168 CD
8	CL	*	.051+- .007	.146+- .035	.054+- .088	1.049+- 2.510 CL
9	CO	*	.003+- .002	.009+- .006	.004+- .000	1.308+- .081 CO
10	CR	*	.002+- .002	.011+- .011	.006+- .000	2.912+- .626 CR
11	CU	*	.013+- .002	.037+- .009	.012+- .002	.957+- .170 CU
12	FE	*	.208+- .011	.594+- .123	.207+- .029	.994+- .197 FE
13	HG	*	< .000	< .009	.004+- .000	.000+- .000 HG
14	K	*	.165+- .009	.471+- .098	.161+- .037	.973+- .314 K
15	MN	*	.022+- .004	.063+- .017	.022+- .003	1.019+- .202 MN
16	NI	*	.006+- .001	.017+- .004	.006+- .000	1.003+- .075 NI
17	P	*	.119+- .017	.340+- .084	.004+- .000	.033+- .001 P
18	PB	*	1.422+- .068	4.063+- .835	1.014+- .245	.713+- .211 PB
19	SO4	*	13.130+- .681	37.514+- 7.751	13.151+- 1.780	1.002+- .192 SO4
20	SB	*	.003+- .002	.009+- .006	.004+- .000	1.479+- .076 SB
21	SI	*	.277+- .031	.791+- .181	.290+- .050	1.045+- .261 SI
22	SN	*	< .001	< .006	.019+- .004	18.516+- 67.641 SN
23	SR	*	.003+- .001	.009+- .003	.004+- .000	1.261+- .019 SR
24	TI	*	.007+- .007	< .040	.005+- .001	.768+- .102 TI
25	V	*	< .002	< .023	.004+- .000	2.080+- .056 V
26	ZN	*	.042+- .003	.120+- .025	.042+- .007	.995+- .247 ZN
27	C	M	< .000	< .003	7.740+- 1.024	.000+- .000 C
28	NA	M	< .000	< .003	-.116+- .035	.000+- .000 NA
29	NO3	M	< .000	< .003	.043+- .009	.000+- .000 NO3
30	RB	M	< .000	< .003	.004+- .000	.000+- .000 RB
31	SE	M	< .000	< .003	.004+- .000	.000+- .000 SE

MEASURED AMBIENT MASS (UG/M3): FINE: 35.0+- 7.0 COARSE: 75.0+- 7.0 TOTAL: 110.0+- 9.9

TABLE C-7 (CONTINUED)

RESULTS FOR CMB SITE: URBAN CORE YEAR: 81 DATE: 0229

COARSE PARTICULATE FRACTION

SAMPLING DURATION: 12 HRS. WITH START HOUR: 7

BACKGROUND SITE SUBTRACTED: NO

CODE	SOURCE	RIDGE REGRESSION			LEAST SQUARES		
		UG/M3	Z		UG/M3	VIF	
	INTERCEPT	.011+- .005			.023+- .010		
1	SOIL	36.445+- 18.752	48.593+-25.410		77.894+- 81.347	6.178	
2	RD DUST	13.578+- 6.185	18.104+- 8.418		18.281+- 13.310	2.184	
3	SEA SALT	.177+- .491	.328+- .655		.365+- .771	1.223	
5	AUTO CAT	10.339+- 13.655	9.126+-18.252		-51.096+- 63.596	6.754	
6	AUTO	.722+- .275	.963+- .378		1.180+- .395	1.054	
9	DIST OIL	.000+- .000	.000+- .000		.000+- .000	.000	
10	RES GAS	.000+- .000	.000+- .000		.000+- .000	.000	
11	COAL	4.532+- 3.137	6.043+- 4.220		11.906+- 7.909	2.829	
12	KRAFT RB	2.229+- 3.455	2.308+- 4.615		-.031+- 6.302	1.564	
13	ELARCFRN	.000+- .000	.000+- .000		.000+- .000	.000	
14	FERRMFR	.000+- .000	.000+- .000		.000+- .000	.000	
16	CEMENT	13.874+- 11.324	18.499+-15.197		23.364+- 20.317	1.550	
17	PET FCC	.000+- .000	.000+- .000		.000+- .000	.000	
19	SEC SO4	.000+- .000	.000+- .000		.000+- .000	.000	
TOTAL:		81.908+- 25.267	109.210+-35.197		81.884+- 43.046		

SPECIES CODE	FIT FLG	MISS FLG	COARSE MEAS. UG/M3	SUSPENDED PERCENT	PARTICULATE CALC. UG/M3	RATIO	
1	TOTAL	*	75.000+- 7.000	100.000+-13.199	81.908+-25.267	1.092+- .499	TOTAL
2	AL	*	1.951+- .422	2.601+- .613	1.125+- .229	.377+- .136	AL
3	AS		.004+- .004	.003+- .005	.011+- .000	2.762+- .000	AS
4	BA	*	.371+- .023	.495+- .055	.011+- .000	.030+- .000	BA
5	BR	*	.108+- .007	.144+- .016	.073+- .015	.672+- .165	BR
6	CA	*	13.014+- 1.442	17.352+- 2.514	5.186+- .842	.399+- .070	CA
7	CD		< .001	< .001	.011+- .000	22.097+- .000	CD
8	CL	*	.288+- .068	.384+- .097	.212+- .031	.736+- .133	CL
9	CO	*	.015+- .003	.020+- .004	.011+- .000	.737+- .035	CO
10	CR	*	.022+- .005	.029+- .007	.022+- .003	.989+- .171	CR
11	CU	*	.018+- .002	.024+- .003	.018+- .001	1.010+- .084	CU
12	FE	*	1.871+- .118	2.495+- .281	1.204+- .205	.643+- .130	FE
13	HG		< .001	< .003	.011+- .000	11.048+- 4.756	HG
14	K	*	.517+- .072	.689+- .116	.347+- .070	.672+- .164	K
15	MN	*	.088+- .008	.117+- .015	.035+- .004	.398+- .048	MN
16	NI		.003+- .001	.004+- .001	.018+- .001	5.834+- 2.534	NI
17	P	*	.102+- .040	.136+- .055	.011+- .000	.108+- .004	P
18	PB	*	.346+- .024	.461+- .054	.171+- .038	.494+- .123	PB
19	SO4		1.725+- .939	2.300+- 1.270	6.525+- 1.306	3.782+- 2.962	SO4
20	SB		.004+- .002	.005+- .003	.011+- .000	2.762+- .000	SB
21	SI	*	8.652+- 1.987	11.536+- 2.860	6.335+- 1.048	.732+- .150	SI
22	SN		.005+- .002	.007+- .003	.011+- .000	2.210+- .000	SN
23	SR	*	.030+- .003	.040+- .005	.016+- .001	.538+- .048	SR
24	TI	*	.205+- .037	.273+- .056	.181+- .035	.881+- .229	TI
25	V		< .007	< .019	.015+- .001	2.102+- .307	V
26	ZN	*	.071+- .006	.095+- .012	.054+- .008	.756+- .142	ZN
27	C	M	< .000	< .001	8.129+- 1.224	.000+- .000	C
28	NA	M	< .000	< .001	.422+- .068	.000+- .000	NA
29	NO3	M	< .000	< .001	.014+- .001	.000+- .000	NO3
30	RB	M	< .000	< .001	.012+- .000	.000+- .000	RB
31	SE	M	< .000	< .001	.011+- .000	.000+- .000	SE

MEASURED AMBIENT MASS (UG/M3): FINE: 35.0+- 7.0 COARSE: 25.0+- 7.0 TOTAL: 110.0+- 9.9

TABLE C-7 (CONTINUED)

RESULTS FOR CMB SITE: URBAN CORE YEAR: 81 DATE: 0229
 TOTAL PARTICULATE FRACTION
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO
 RESULTS DERIVED FROM FINE AND COARSE FITTINGS

CODE	SOURCE	UG/M3		Z
	INTERCEPT	.015+-	.006	
1	SOIL	35.936+-	19.005	32.669+-17.525
2	RD DUST	13.554+-	6.254	12.321+- 5.792
3	SEA SALT	-.270+-	.520	.237+- .473
5	AUTO CAT	17.717+-	24.579	11.196+-22.391
6	AUTO	5.358+-	.980	4.871+- .993
9	DIST OIL	3.596+-	6.614	3.010+- 6.020
10	RES GAS	1.015+-	5.311	2.415+- 4.829
11	COAL	6.303+-	3.414	5.730+- 3.146
12	KRAFT RB	2.229+-	3.455	1.573+- 3.146
13	ELARCFRN	.076+-	.454	.206+- .412
14	FERRMFR	.061+-	.250	.114+- .227
16	CEMENT	21.277+-	11.694	19.343+-10.773
17	PET FCC	8.221+-	12.252	5.579+-11.159
19	SEC S04	-.187+-	11.012	5.006+-10.011
TOTAL:		114.899+-	29.467	104.454+-28.390

SPECIES CODE	FIT	MISS	TOTAL	SUSPENDED PARTICULATE		RATIO	
	FLG	FLG	MEAS. UG/M3	PERCENT	CALC. UG/M3		
1	TOTAL	*	110.000+-	9.899	100.000+-12.727	114.899+-29.467	1.045+- .387 TOTAL
2	AL	*	2.039+-	.427	1.854+- .422	1.154+- .229	.566+- .129 AL
3	AS		.040+-	.008	.036+- .008	.015+- .000	.374+- .000 AS
4	BA	*	.520+-	.027	.473+- .049	.015+- .000	.029+- .000 BA
5	BR	*	.452+-	.018	.411+- .041	.458+- .096	1.013+- .303 BR
6	CA	*	13.455+-	1.442	12.232+- 1.712	5.627+- .847	.418+- .068 CA
7	CD		.004+-	.002	.004+- .002	.017+- .000	3.677+- .334 CD
8	CL	*	.339+-	.068	.308+- .068	.266+- .094	.783+- .350 CL
9	CO	*	.018+-	.004	.016+- .004	.015+- .000	.832+- .033 CO
10	CR	*	.024+-	.006	.022+- .006	.028+- .003	1.149+- .172 CR
11	CU	*	.031+-	.003	.028+- .004	.031+- .002	.988+- .087 CU
12	FE	*	2.079+-	.119	1.890+- .201	1.411+- .207	.679+- .120 FE
13	HG		< .001	< .003	< .003	.015+- .000	14.973+- 6.801 HG
14	K	*	.682+-	.073	.620+- .086	.508+- .079	.745+- .145 K
15	MN	*	.110+-	.009	.100+- .012	.057+- .005	.322+- .051 MN
16	NI		.009+-	.001	.008+- .001	.024+- .001	2.613+- .411 NI
17	P	*	.221+-	.043	.201+- .043	.015+- .000	.068+- .002 P
18	PB	*	1.768+-	.072	1.607+- .159	1.184+- .248	.670+- .169 PB
19	S04		14.855+-	1.160	13.505+- 1.609	19.676+- 2.208	1.325+- .247 S04
20	SB		.007+-	.003	.006+- .003	.015+- .000	2.212+- .044 SB
21	SI	*	8.929+-	1.987	8.117+- 1.949	6.624+- 1.050	.742+- .146 SI
22	SN		.006+-	.003	.005+- .003	.030+- .004	4.927+- 3.057 SN
23	SR	*	.033+-	.003	.030+- .004	.020+- .001	.604+- .045 SR
24	TI	*	.212+-	.040	.193+- .040	.186+- .035	.877+- .221 TI
25	V		< .009	< .015	< .015	.019+- .001	2.097+- .239 V
26	ZN	*	.113+-	.007	.103+- .011	.095+- .011	.845+- .126 ZN
27	C	M	< .000	< .001	< .001	15.870+- 1.596	.000+- .000 C
28	NA	M	< .000	< .001	< .001	.305+- .076	.000+- .000 NA
29	NO3	M	< .000	< .001	< .001	.057+- .009	.000+- .000 NO3
30	RB	M	< .000	< .001	< .001	.016+- .000	.000+- .000 RB
31	SE	M	< .000	< .001	< .001	.015+- .000	.000+- .000 SE

MEASURED AMBIENT MASS (UG/M3): FINE: 35.0+- 7.0 COARSE: 75.0+- 7.0 TOTAL: 110.0+- 9.9

TABLE C-7 (CONTINUED)

RESULTS FOR CNB SITE: BACKGROUND YEAR: 81 DATE: 0229
 FINE PARTICULATE FRACTION
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO

CODE	SOURCE	RIDGE REGRESSION		LEAST SQUARES	
		UG/M3	Z	UG/M3	VIF
	INTERCEPT	.006+- .006		.005+- .006	
1	SOIL	-.334+- .346	.622+- 1.243	-14.654+- 34.854	7594.633
2	RD DUST	.214+- .656	1.171+- 2.343	1.231+- 3.814	91.330
3	SEA SALT	-.187+- .093	.170+- .341	-.667+- .264	19.554
5	AUTO CAT	12.538+- 7.325	44.778+- 26.596	-26.438+- 39.874	52.511
6	AUTO	1.889+- .609	6.745+- 2.291	2.261+- .522	1.823
9	DIST OIL	1.572+- 3.786	6.768+- 13.536	20.923+- 12.055	25.512
10	RES GAS	-.735+- .733	1.316+- 2.632	17.660+- 61.095	6725.402
11	COAL	1.088+- .951	3.887+- 3.420	3.035+- 2.132	13.675
13	ELARCFRN	-.053+- .114	.204+- .408	-.117+- .974	93.757
14	FERRMFR	.147+- .137	.523+- .492	.186+- .498	22.554
16	CEMENT	2.884+- 1.166	10.300+- 4.307	9.390+- 3.855	30.223
17	PET FCC	4.596+- 4.504	16.416+- 16.183	6.337+- 24.170	55.903
19	SEC S04	4.025+- 4.481	8.038+- 16.076	7.995+- 30.701	78.138
TOTAL:		27.650+- 7.882	98.750+- 30.073	27.147+- 20.851	

SPECIES CODE	FIT FLG	MISS FLG	MEAS. UG/M3	FINE SUSPENDED PARTICULATE PERCENT	CALC. UG/M3	RATIO
1	TOTAL	*	28.000+- 3.000	100.000+- 15.152	27.650+- 7.882	.988+- .396 TOTAL
2	AL	*	.070+- .055	.250+- .198	.048+- .006	.692+- .110 AL
3	AS	*	.014+- .006	.050+- .022	.006+- .000	.403+- .000 AS
4	BA	*	.146+- .018	.521+- .085	.006+- .000	.040+- .000 BA
5	BR	*	.164+- .010	.586+- .072	.161+- .039	.983+- .331 BR
6	CA	*	.128+- .008	.457+- .057	.133+- .039	1.039+- .437 CA
7	CD	*	< .001	< .007	.007+- .000	6.613+- 1.623 CD
8	CL	*	.010+- .007	.036+- .025	.023+- .037	2.319+- 9.227 CL
9	CO	*	.008+- .003	.029+- .011	.006+- .000	.705+- .022 CO
10	CR	*	.010+- .005	.036+- .018	.005+- .000	.487+- .031 CR
11	CU	*	.027+- .003	.096+- .015	.011+- .001	.426+- .041 CU
12	FE	*	.120+- .008	.429+- .054	.116+- .018	.963+- .205 FE
13	HG	*	< .001	< .011	.006+- .000	3.763+- .377 HG
14	K	*	.186+- .010	.664+- .080	.086+- .015	.461+- .089 K
15	MN	*	.022+- .004	.079+- .017	.029+- .006	1.303+- .482 MN
16	NI	*	.003+- .002	.011+- .007	.007+- .000	2.463+- .421 NI
17	P	*	.103+- .018	.368+- .075	.006+- .000	.055+- .001 P
18	PB	*	.894+- .047	3.193+- .381	.420+- .100	.470+- .123 PB
19	S04	*	14.780+- .765	52.786+- 6.281	14.288+- 1.728	.967+- .163 S04
20	SB	*	.008+- .003	.029+- .011	.006+- .000	.745+- .012 SB
21	SI	*	.189+- .027	.675+- .121	.225+- .029	1.188+- .236 SI
22	SN	*	.024+- .003	.086+- .014	.015+- .002	.609+- .109 SN
23	SR	*	.003+- .002	.011+- .007	.006+- .000	1.850+- .016 SR
24	TI	*	< .008	< .057	.008+- .000	.978+- .086 TI
25	V	*	< .003	< .032	.006+- .000	1.925+- .019 V
26	ZN	*	.038+- .003	.136+- .018	.035+- .005	.911+- .181 ZN
27	C	M	< .000	< .004	6.858+- 1.259	.000+- .000 C
28	NA	M	< .000	< .004	-.038+- .015	.000+- .000 NA
29	NO3	M	< .000	< .004	.030+- .004	.000+- .000 NO3
30	RB	M	< .000	< .004	.006+- .000	.000+- .000 RB
31	SE	M	< .000	< .004	.006+- .000	.000+- .000 SE

MEASURED AMBIENT MASS (UG/M3): FINE: 28.0+- 3.0 COARSE: 37.0+- 4.0 TOTAL: 65.0+- 5.0

TABLE C-7 (CONTINUED)

RESULTS FOR CMB SITE: BACKGROUND YEAR: 81 DATE: 0229

COARSE PARTICULATE FRACTION

SAMPLING DURATION: 12 HRS. WITH START HOUR: 7

BACKGROUND SITE SUBTRACTED: NO

RIDGE REGRESSION

K= .480

R-SQUARE: .8785

LEAST SQUARES

K=0.0

R-SQUARE: .9570

CODE	SOURCE	UG/M3		Z	UG/M3		VIF
	INTERCEPT	.003+-	.002		.003+-	.003	
1	SOIL	20.253+-	5.861	54.738+-16.911	27.211+-	16.919	7.651
2	RD DUST	6.130+-	1.363	16.567+- 4.097	7.989+-	2.435	3.687
3	SEA SALT	-.024+-	.031	.042+- .084	-.053+-	.114	10.065
5	AUTO CAT	1.749+-	4.822	6.522+-13.043	-9.926+-	14.544	8.157
6	AUTO	.540+-	.106	1.460+- .327	.820+-	.099	1.130
9	DIST OIL	.000+-	.000	.000+- .000	.000+-	.000	.000
10	RES GAS	.000+-	.000	.000+- .000	.000+-	.000	.000
11	COAL	1.397+-	.840	3.775+- 2.307	2.655+-	1.708	4.580
12	KRAFT RB	.053+-	.538	.726+- 1.453	-.156+-	2.073	10.701
13	ELARCFRN	.000+-	.000	.000+- .000	.000+-	.000	.000
14	FERRMFR	.000+-	.000	.000+- .000	.000+-	.000	.000
16	CEMENT	6.954+-	2.694	18.796+- 7.558	9.610+-	3.288	1.852
17	PET FCC	.000+-	.000	.000+- .000	.000+-	.000	.000
19	SEC S04	.000+-	.000	.000+- .000	.000+-	.000	.000
TOTAL:		37.055+-	13.502	100.148+-38.064	38.153+-	21.236	

SPECIES CODE	FIT FLG	MISS FLG	COARSE SUSPENDED PARTICULATE				RATIO	
			MEAS. UG/M3	PERCENT	CALC. UG/M3			
1	TOTAL	*	37.000+- 4.000	100.000+-15.289	37.055+-13.502	1.001+-	.516	TOTAL
2	AL	*	.739+- .171	1.997+- .510	.521+- .105	.705+-	.173	AL
3	AS		< .001	< .011	.003+- .000	2.948+-	.000	AS
4	BA	*	.086+- .016	.232+- .050	.003+- .000	.034+-	.000	BA
5	BR	*	.064+- .005	.173+- .023	.048+- .011	.746+-	.216	BR
6	CA	*	3.805+- .444	10.284+- 1.636	2.646+- .436	.696+-	.139	CA
7	CD		.001	< .005	.003+- .000	2.948+-	.000	CD
8	CL	*	.014+- .010	.038+- .027	.020+- .008	1.460+-	1.013	CL
9	CO	*	< .001	< .008	.003+- .000	2.948+-	.697	CO
10	CR	*	< .003	< .014	.003+- .000	1.281+-	.041	CR
11	CU	*	.004+- .002	.011+- .006	.005+- .000	1.311+-	.189	CU
12	FE	*	.692+- .044	1.870+- .235	.513+- .092	.741+-	.166	FE
13	HG		.009+- .003	.024+- .009	.003+- .000	.328+-	.026	HG
14	K	*	.215+- .032	.581+- .107	.167+- .035	.777+-	.208	K
15	MN	*	.018+- .004	.049+- .012	.014+- .002	.757+-	.130	MN
16	NI		.001	< .005	.003+- .000	3.327+-	.247	NI
17	P	*	< .020	< .060	.003+- .000	.147+-	.011	P
18	PB	*	.213+- .017	.576+- .077	.121+- .029	.568+-	.154	PB
19	S04		.852+- .783	2.303+- 2.131	1.315+- .229	1.544+-	.495	S04
20	SB		.001	< .008	.003+- .000	2.948+-	.000	SB
21	SI	*	4.000+- .914	10.811+- 2.733	2.981+- .484	.745+-	.151	SI
22	SN		.003+- .003	.004+- .008	.003+- .000	.983+-	.000	SN
23	SR	*	.006+- .002	.016+- .006	.006+- .001	.964+-	.164	SR
24	TI	*	.097+- .017	.262+- .054	.083+- .016	.854+-	.219	TI
25	V		< .003	< .019	.005+- .000	1.315+-	.197	V
26	ZN	*	.016+- .003	.043+- .009	.016+- .002	.989+-	.216	ZN
27	C	M	< .000	< .003	2.610+- .386	.000+-	.000	C
28	NA	M	< .000	< .003	.106+- .027	.000+-	.000	NA
29	NO3	M	< .000	< .003	.004+- .000	.000+-	.000	NO3
30	RB	M	< .000	< .003	.003+- .000	.000+-	.000	RB
31	SE	M	< .000	< .003	.003+- .000	.000+-	.000	SE

MEASURED AMBIENT MASS (UG/M3): FINE: 28.0+- 3.0 COARSE: 37.0+- 4.0 TOTAL: 65.0+- 5.0

TABLE C-7 (CONTINUED)

RESULTS FOR CMB SITE: BACKGROUND YEAR: 81 DATE: 0229
 TOTAL PARTICULATE FRACTION
 SAMPLING DURATION: 12 HRS. WITH START HOUR: 7
 BACKGROUND SITE SUBTRACTED: NO
 RESULTS DERIVED FROM FINE AND COARSE FITTINGS

CODE	SOURCE	UG/M3		Z
	INTERCEPT	.009+-	.006	
1	SOIL	19.919+-	5.872	30.645+- 9.336
2	RD DUST	6.343+-	1.513	9.759+- 2.445
3	SEA SALT	-.211+-	.098	.077+- .153
5	AUTO CAT	14.287+-	8.770	21.980+-13.597
6	AUTO	2.429+-	.618	3.736+- .993
9	DIST OIL	1.572+-	3.786	2.914+- 5.828
10	RES GAS	-.735+-	.733	.565+- 1.131
11	COAL	2.485+-	1.269	3.823+- 1.974
12	KRAFT RB	.053+-	.538	.413+- .827
13	ELARCFRN	-.053+-	.114	.088+- .176
14	FERRMFR	.147+-	.137	.225+- .211
16	CEMENT	9.838+-	2.935	15.136+- 4.663
17	PET FCC	4.596+-	4.504	7.071+- 6.951
19	SEC SO4	4.025+-	4.481	3.455+- 6.910
TOTAL:		64.705+-	15.634	99.546+-25.242

SPECIES CODE	FIT FLG	MISS FLG	TOTAL MEAS. UG/M3	SUSPENDED PARTICULATE PERCENT	CALC. UG/M3	RATIO
1	TOTAL	*	65.000+-	5.000	100.000+-10.879	64.705+-15.634 .995+- .339 TOTAL
2	AL	*	.809+-	.180	1.245+- .292	.569+- .105 .704+- .159 AL
3	AS	*	.015+-	.007	.023+- .011	.009+- .000 .573+- .000 AS
4	BA	*	.232+-	.024	.357+- .046	.009+- .000 .038+- .000 BA
5	BR	*	.228+-	.011	.351+- .032	.209+- .040 .916+- .240 BR
6	CA	*	3.933+-	.444	6.051+- .827	2.780+- .437 .707+- .136 CA
7	CD	*	<	.002	< .004	.010+- .000 4.780+- .593 CD
8	CL	*	.024+-	.012	.037+- .019	.044+- .037 1.818+- 3.233 CL
9	CO	*	.009+-	.004	.014+- .007	.009+- .000 .955+- .041 CO
10	CR	*	.012+-	.007	.019+- .011	.008+- .000 .646+- .027 CR
11	CU	*	.031+-	.004	.048+- .007	.017+- .001 .540+- .041 CU
12	FE	*	.812+-	.045	1.249+- .118	.628+- .094 .774+- .146 FE
13	HG	*	.010+-	.004	.016+- .007	.009+- .000 .818+- .033 HG
14	K	*	.401+-	.034	.617+- .070	.253+- .038 .631+- .113 K
15	MN	*	.040+-	.006	.062+- .010	.042+- .007 1.057+- .245 MN
16	NI	*	.004+-	.003	.006+- .004	.011+- .000 2.679+- .343 NI
17	P	*	.123+-	.028	.189+- .046	.009+- .000 .070+- .002 P
18	PB	*	1.107+-	.050	1.703+- .152	.541+- .104 .489+- .104 PB
19	SO4	*	15.632+-	1.095	24.049+- 2.502	15.603+- 1.743 .998+- .158 SO4
20	SB	*	.009+-	.004	.014+- .007	.009+- .000 .990+- .012 SB
21	SI	*	4.189+-	.914	6.445+- 1.492	3.205+- .485 .765+- .146 SI
22	SN	*	.027+-	.004	.042+- .007	.018+- .002 .650+- .099 SN
23	SR	*	.009+-	.003	.014+- .004	.011+- .001 1.259+- .127 SR
24	TI	*	.105+-	.023	.162+- .038	.091+- .016 .864+- .203 TI
25	V	*	<	.006	< .018	.010+- .000 1.596+- .121 V
26	ZN	*	.054+-	.004	.083+- .009	.050+- .006 .934+- .143 ZN
27	C	M	<	.000	< .002	9.468+- 1.317 .000+- .000 C
28	NA	M	<	.000	< .002	.067+- .031 .000+- .000 NA
29	NO3	M	<	.000	< .002	.034+- .004 .000+- .000 NO3
30	RB	M	<	.000	< .002	.009+- .000 .000+- .000 RB
31	SE	M	<	.000	< .002	.009+- .000 .000+- .000 SE

MEASURED AMBIENT MASS (UG/M3): FINE: 28.0+- 3.0 COARSE: 37.0+- 4.0 TOTAL: 65.0+- 5.0

TABLE C-7 (CONTINUED)

RIDGE K	.000	.005	.010	.015	.020	.025	.030
INTERCEPT	.004+- .003	.004+- .003	.004+- .002	.004+- .002	.004+- .002	.004+- .002	.004+- .002
SOIL	22.079+-19.624	21.180+-17.940	20.448+-16.547	19.828+-15.377	19.299+-14.382	18.844+-13.527	18.449+-12.785
RD DUST	8.616+- 3.282	8.667+- 3.164	8.701+- 3.066	8.722+- 2.984	8.734+- 2.916	8.739+- 2.857	8.737+- 2.805
SEA SALT	-.054+- .120	-.052+- .115	-.050+- .110	-.049+- .105	-.048+- .101	-.047+- .098	-.046+- .094
AUTO CAT	-6.547+-16.549	-5.666+-15.120	-4.919+-13.942	-4.267+-12.949	-3.692+-12.102	-3.181+-11.371	-2.723+-10.735
AUTO	.847+- .286	.841+- .282	.836+- .278	.831+- .275	.825+- .272	.820+- .269	.815+- .266
COAL	2.268+- 2.178	2.174+- 2.022	2.093+- 1.896	2.021+- 1.790	1.958+- 1.699	1.902+- 1.620	1.851+- 1.552
KRAFT RB	-.203+- 1.980	-.220+- 1.894	-.234+- 1.815	-.245+- 1.743	-.254+- 1.677	-.260+- 1.616	-.266+- 1.559
CEMENT	10.305+- 5.092	10.365+- 4.964	10.399+- 4.842	10.419+- 4.735	10.427+- 4.641	10.425+- 4.557	10.415+- 4.481
RIDGE K	.035	.040	.045	.050	.060	.070	.080
INTERCEPT	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002
SOIL	18.106+-12.136	17.806+-11.565	17.542+-11.059	17.309+-10.608	16.920+- 9.841	16.609+- 9.214	16.360+- 8.692
RD DUST	8.730+- 2.759	8.720+- 2.719	8.706+- 2.682	8.689+- 2.648	8.648+- 2.588	8.601+- 2.536	8.549+- 2.490
SEA SALT	-.045+- .091	-.044+- .088	-.043+- .085	-.042+- .082	-.041+- .078	-.040+- .073	-.039+- .069
AUTO CAT	-2.310+-10.177	-1.936+- 9.684	-1.596+- 9.246	-1.284+- 8.854	-.735+- 8.184	-.264+- 7.637	.144+- 7.178
AUTO	.810+- .263	.805+- .260	.800+- .257	.795+- .255	.785+- .250	.776+- .245	.767+- .240
COAL	1.805+- 1.492	1.763+- 1.439	1.725+- 1.392	1.690+- 1.350	1.627+- 1.278	1.574+- 1.219	1.527+- 1.170
KRAFT RB	-.270+- 1.506	-.272+- 1.457	-.274+- 1.411	-.275+- 1.368	-.276+- 1.290	-.274+- 1.221	-.271+- 1.160
CEMENT	10.399+- 4.411	10.378+- 4.346	10.353+- 4.286	10.325+- 4.229	10.260+- 4.125	10.189+- 4.032	10.113+- 3.948
RIDGE K	.090	.100	.120	.140	.160	.180	.200
INTERCEPT	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002
SOIL	16.158+- 8.252	15.993+- 7.878	15.742+- 7.274	15.567+- 6.810	15.441+- 6.443	15.349+- 6.147	15.279+- 5.904
RD DUST	8.494+- 2.448	8.437+- 2.411	8.320+- 2.344	8.200+- 2.286	8.081+- 2.235	7.963+- 2.190	7.848+- 2.150
SEA SALT	-.037+- .066	-.037+- .063	-.035+- .058	-.033+- .054	-.032+- .050	-.031+- .047	-.029+- .045
AUTO CAT	.501+- 6.792	.817+- 6.462	1.351+- 5.930	1.785+- 5.522	2.147+- 5.201	2.453+- 4.943	2.715+- 4.733
AUTO	.758+- .236	.749+- .232	.732+- .225	.716+- .218	.701+- .212	.687+- .206	.673+- .201
COAL	1.486+- 1.128	1.449+- 1.092	1.387+- 1.034	1.335+- .990	1.292+- .954	1.255+- .925	1.223+- .902
KRAFT RB	-.267+- 1.105	-.262+- 1.055	-.252+- .971	-.240+- .901	-.228+- .843	-.216+- .794	-.204+- .752
CEMENT	10.035+- 3.870	9.955+- 3.799	9.794+- 3.672	9.635+- 3.562	9.480+- 3.465	9.329+- 3.380	9.184+- 3.305
RIDGE K	.240	.280	.320	.360	.400	.480	.560
INTERCEPT	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.003+- .002	.002+- .002
SOIL	15.178+- 5.531	15.109+- 5.261	15.054+- 5.059	15.004+- 4.905	14.955+- 4.785	14.845+- 4.615	14.727+- 4.505
RD DUST	7.626+- 2.082	7.416+- 2.024	7.218+- 1.976	7.030+- 1.934	6.853+- 1.898	6.527+- 1.838	6.234+- 1.788
SEA SALT	-.027+- .041	-.025+- .037	-.024+- .035	-.022+- .033	-.021+- .032	-.018+- .030	-.016+- .029
AUTO CAT	3.143+- 4.413	3.474+- 4.185	3.738+- 4.018	3.952+- 3.892	4.128+- 3.797	4.397+- 3.664	4.584+- 3.583
AUTO	.647+- .192	.624+- .184	.602+- .178	.582+- .172	.564+- .167	.531+- .159	.502+- .152
COAL	1.170+- .865	1.128+- .839	1.094+- .819	1.065+- .804	1.040+- .792	1.001+- .775	.970+- .764
KRAFT RB	-.181+- .686	-.159+- .636	-.139+- .598	-.120+- .568	-.103+- .545	-.072+- .511	-.046+- .488
CEMENT	8.910+- 3.179	8.655+- 3.076	8.419+- 2.992	8.199+- 2.921	7.993+- 2.862	7.619+- 2.769	7.284+- 2.695
RIDGE K	.640	.720	.800				
INTERCEPT	.002+- .002	.002+- .002	.002+- .002				
SOIL	14.595+- 4.431	14.452+- 4.380	14.300+- 4.343				
RD DUST	5.967+- 1.746	5.725+- 1.708	5.502+- 1.674				
SEA SALT	-.015+- .028	-.013+- .027	-.012+- .026				
AUTO CAT	4.717+- 3.532	4.811+- 3.500	4.875+- 3.479				
AUTO	.476+- .146	.454+- .141	.433+- .137				
COAL	.945+- .756	.925+- .750	.908+- .744				
KRAFT RB	-.023+- .473	-.003+- .462	.014+- .454				
CEMENT	6.983+- 2.636	6.710+- 2.586	6.460+- 2.542				

TABLE C-8. USER FOLLOWUP OUTPUT FILE

3 URBAN CORE	810229	12	7	12				
30 URBAN CORE	810229	12	7	1	35.0000	7.0000	75.0000	7.0000
30 URBAN CORE	810229	12	7	2	.0880	.0620	1.9510	.4220
30 URBAN CORE	810229	12	7	3	.0360	.0070	.0040	.0040
30 URBAN CORE	810229	12	7	4	.1490	.0140	.3710	.0230
30 URBAN CORE	810229	12	7	5	.3440	.0170	.1080	.0070
30 URBAN CORE	810229	12	7	6	.4410	.0230	13.0140	1.4420
30 URBAN CORE	810229	12	7	7	.0040	.0020	.0005	.0010
30 URBAN CORE	810229	12	7	8	.0510	.0070	.2880	.0680
30 URBAN CORE	810229	12	7	9	.0030	.0020	.0150	.0030
30 URBAN CORE	810229	12	7	10	.0020	.0040	.0220	.0050
30 URBAN CORE	810229	12	7	11	.0130	.0020	.0180	.0020
30 URBAN CORE	810229	12	7	12	.2080	.0110	1.8710	.1180
30 URBAN CORE	810229	12	7	13	.0000	.0030	.0010	.0020
30 URBAN CORE	810229	12	7	14	.1650	.0090	.5170	.0720
30 URBAN CORE	810229	12	7	15	.0220	.0040	.0880	.0080
30 URBAN CORE	810229	12	7	16	.0060	.0010	.0030	.0010
30 URBAN CORE	810229	12	7	17	.1190	.0170	.1020	.0400
30 URBAN CORE	810229	12	7	18	1.4220	.0680	.3460	.0240
30 URBAN CORE	810229	12	7	19	13.1300	.6810	1.7250	.9390
30 URBAN CORE	810229	12	7	20	.0030	.0020	.0040	.0020
30 URBAN CORE	810229	12	7	21	.2770	.0310	8.6520	1.9870
30 URBAN CORE	810229	12	7	22	.0010	.0020	.0050	.0020
30 URBAN CORE	810229	12	7	23	.0030	.0010	.0300	.0030
30 URBAN CORE	810229	12	7	24	.0070	.0140	.2050	.0370
30 URBAN CORE	810229	12	7	25	.0020	.0080	.0070	.0140
30 URBAN CORE	810229	12	7	26	.0420	.0030	.0710	.0060
3 URBAN CORE	810229	12	7	12				
30 URBAN CORE	810229	12	7	1	35.0000	7.0000	75.0000	7.0000
30 URBAN CORE	810229	12	7	2	.0880	.0620	1.9510	.4220
30 URBAN CORE	810229	12	7	3	.0360	.0070	.0040	.0040
30 URBAN CORE	810229	12	7	4	.1490	.0140	.3710	.0230
30 URBAN CORE	810229	12	7	5	.3440	.0170	.1080	.0070
30 URBAN CORE	810229	12	7	6	.4410	.0230	13.0140	1.4420
30 URBAN CORE	810229	12	7	7	.0040	.0020	.0005	.0010
30 URBAN CORE	810229	12	7	8	.0510	.0070	.2880	.0680
30 URBAN CORE	810229	12	7	9	.0030	.0020	.0150	.0030
30 URBAN CORE	810229	12	7	10	.0020	.0040	.0220	.0050
30 URBAN CORE	810229	12	7	11	.0130	.0020	.0180	.0020
30 URBAN CORE	810229	12	7	12	.2080	.0110	1.8710	.1180
30 URBAN CORE	810229	12	7	13	.0000	.0030	.0010	.0020
30 URBAN CORE	810229	12	7	14	.1650	.0090	.5170	.0720
30 URBAN CORE	810229	12	7	15	.0220	.0040	.0880	.0080
30 URBAN CORE	810229	12	7	16	.0060	.0010	.0030	.0010
30 URBAN CORE	810229	12	7	17	.1190	.0170	.1020	.0400

TABLE C-8 (CONTINUED)

30 URBAN CORE	810229	12	7	18	1.4220	.0680	.3460	.0240
30 URBAN CORE	810229	12	7	19	13.1300	.6810	1.7250	.9390
30 URBAN CORE	810229	12	7	20	.0030	.0020	.0040	.0020
30 URBAN CORE	810229	12	7	21	.2770	.0310	8.6520	1.9870
30 URBAN CORE	810229	12	7	22	.0010	.0020	.0050	.0020
30 URBAN CORE	810229	12	7	23	.0030	.0010	.0300	.0030
30 URBAN CORE	810229	12	7	24	.0070	.0140	.2050	.0370
30 URBAN CORE	810229	12	7	25	.0020	.0080	.0070	.0140
30 URBAN CORE	810229	12	7	26	.0420	.0030	.0710	.0060
40 URBAN CORE	810229	12	7	1 1	-.5088	3.0917	36.4449	18.7516
40 URBAN CORE	810229	12	7	1 2	-.0033	.0207	.2004	.1175
40 URBAN CORE	810229	12	7	1 6	-.0473	.2966	1.8587	1.0898
40 URBAN CORE	810229	12	7	1 11	-.0002	.0010	.0033	.0019
40 URBAN CORE	810229	12	7	1 12	-.0042	.0265	.1749	.1026
40 URBAN CORE	810229	12	7	1 14	-.0010	.0064	.0437	.0256
40 URBAN CORE	810229	12	7	1 15	-.0002	.0012	.0077	.0045
40 URBAN CORE	810229	12	7	1 18	-.0001	.0004	.0073	.0043
40 URBAN CORE	810229	12	7	1 19	-.0023	.0144	.0984	.0577
40 URBAN CORE	810229	12	7	1 21	-.0122	.0765	.8747	.5128
40 URBAN CORE	810229	12	7	1 23	-.0001	.0009	.0051	.0030
40 URBAN CORE	810229	12	7	1 24	-.0007	.0045	.0324	.0190
40 URBAN CORE	810229	12	7	1 26	-.0001	.0007	.0033	.0019
40 URBAN CORE	810229	12	7	1 30	.0000	.0001	.0007	.0004
40 URBAN CORE	810229	12	7	2 1	-.0244	.9225	13.5780	6.1852
40 URBAN CORE	810229	12	7	2 2	-.0022	.0841	.8948	.4760
40 URBAN CORE	810229	12	7	2 5	.0000	.0002	.0011	.0006
40 URBAN CORE	810229	12	7	2 6	-.0006	.0232	.4073	.2167
40 URBAN CORE	810229	12	7	2 10	.0000	.0004	.0000	.0000
40 URBAN CORE	810229	12	7	2 11	.0000	.0003	.0000	.0000
40 URBAN CORE	810229	12	7	2 12	-.0015	.0571	.7780	.4139
40 URBAN CORE	810229	12	7	2 14	-.0003	.0098	.0000	.0000
40 URBAN CORE	810229	12	7	2 15	.0000	.0012	.0136	.0072
40 URBAN CORE	810229	12	7	2 16	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	2 18	-.0001	.0035	.0000	.0000
40 URBAN CORE	810229	12	7	2 19	-.0003	.0106	.0000	.0000
40 URBAN CORE	810229	12	7	2 21	-.0054	.2121	3.8561	2.0513
40 URBAN CORE	810229	12	7	2 24	-.0002	.0061	.1371	.0730
40 URBAN CORE	810229	12	7	2 25	.0000	.0002	.0037	.0020
40 URBAN CORE	810229	12	7	2 26	.0000	.0010	.0000	.0000
40 URBAN CORE	810229	12	7	2 27	-.0033	.1298	.6640	.3532
40 URBAN CORE	810229	12	7	2 28	-.0003	.0119	.2376	.1264
40 URBAN CORE	810229	12	7	2 29	.0000	.0000	.0027	.0014
40 URBAN CORE	810229	12	7	3 1	-.4464	.1712	.1769	.4910
40 URBAN CORE	810229	12	7	3 6	-.0045	.0021	.0018	.0051
40 URBAN CORE	810229	12	7	3 8	-.2455	.1148	.0973	.2794
40 URBAN CORE	810229	12	7	3 14	-.0045	.0021	.0018	.0051
40 URBAN CORE	810229	12	7	3 19	-.0402	.0188	.0159	.0457

TABLE C-8 (CONTINUED)

40 URBAN CORE	810229	12	7	3	28	-.1384	.0647	.0548	.1575
40 URBAN CORE	810229	12	7	5	1	7.3772	20.4363	10.3394	13.6553
40 URBAN CORE	810229	12	7	5	2	.0089	.0254	.0124	.0172
40 URBAN CORE	810229	12	7	5	6	.0125	.0359	.0176	.0243
40 URBAN CORE	810229	12	7	5	11	.0018	.0051	.0025	.0034
40 URBAN CORE	810229	12	7	5	12	.0081	.0233	.0114	.0157
40 URBAN CORE	810229	12	7	5	14	.0032	.0093	.0045	.0063
40 URBAN CORE	810229	12	7	5	15	.0011	.0032	.0016	.0021
40 URBAN CORE	810229	12	7	5	16	.0011	.0032	.0016	.0021
40 URBAN CORE	810229	12	7	5	19	3.6886	10.5729	5.1697	7.1555
40 URBAN CORE	810229	12	7	5	21	.0376	.1078	.0527	.0730
40 URBAN CORE	810229	12	7	5	26	.0059	.0169	.0083	.0114
40 URBAN CORE	810229	12	7	5	27	2.8771	8.2469	4.0324	5.5813
40 URBAN CORE	810229	12	7	6	1	4.6355	.9405	.7224	.2752
40 URBAN CORE	810229	12	7	6	2	.0020	.0007	.0003	.0001
40 URBAN CORE	810229	12	7	6	5	.3801	.1239	.0592	.0276
40 URBAN CORE	810229	12	7	6	8	.2503	.0816	.0390	.0182
40 URBAN CORE	810229	12	7	6	11	.0002	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	6	12	.0116	.0038	.0018	.0008
40 URBAN CORE	810229	12	7	6	18	.9781	.3188	.1524	.0710
40 URBAN CORE	810229	12	7	6	19	.0097	.0032	.0015	.0007
40 URBAN CORE	810229	12	7	6	21	.0035	.0011	.0005	.0003
40 URBAN CORE	810229	12	7	6	26	.0010	.0003	.0002	.0001
40 URBAN CORE	810229	12	7	6	27	2.5263	.8235	.3937	.1833
40 URBAN CORE	810229	12	7	9	1	3.5958	6.6142	.0000	.0000
40 URBAN CORE	810229	12	7	9	2	.0111	.0213	.0000	.0000
40 URBAN CORE	810229	12	7	9	5	.0009	.0018	.0000	.0000
40 URBAN CORE	810229	12	7	9	6	.0180	.0344	.0000	.0000
40 URBAN CORE	810229	12	7	9	8	.0431	.0825	.0000	.0000
40 URBAN CORE	810229	12	7	9	11	.0061	.0117	.0000	.0000
40 URBAN CORE	810229	12	7	9	12	.0043	.0083	.0000	.0000
40 URBAN CORE	810229	12	7	9	14	.0006	.0012	.0000	.0000
40 URBAN CORE	810229	12	7	9	15	.0005	.0010	.0000	.0000
40 URBAN CORE	810229	12	7	9	16	.0003	.0006	.0000	.0000
40 URBAN CORE	810229	12	7	9	18	.0194	.0371	.0000	.0000
40 URBAN CORE	810229	12	7	9	19	.4746	.9077	.0000	.0000
40 URBAN CORE	810229	12	7	9	21	.0097	.0186	.0000	.0000
40 URBAN CORE	810229	12	7	9	25	.0002	.0003	.0000	.0000
40 URBAN CORE	810229	12	7	9	26	.0010	.0020	.0000	.0000
40 URBAN CORE	810229	12	7	9	27	1.2873	2.4619	.0000	.0000
40 URBAN CORE	810229	12	7	9	28	.0115	.0220	.0000	.0000
40 URBAN CORE	810229	12	7	9	29	.0360	.0688	.0000	.0000
40 URBAN CORE	810229	12	7	10	1	1.0147	5.3113	.0000	.0000
40 URBAN CORE	810229	12	7	10	6	.0507	.2740	.0000	.0000
40 URBAN CORE	810229	12	7	10	19	.4769	2.5759	.0000	.0000

TABLE C-8 (CONTINUED)

40 URBAN CORE	810229	12	7	10	27	.1218	.6577	.0000	.0000
40 URBAN CORE	810229	12	7	11	1	1.7708	1.3477	4.5322	3.1369
40 URBAN CORE	810229	12	7	11	2	.0078	.0064	.0000	.0000
40 URBAN CORE	810229	12	7	11	4	.0002	.0002	.0000	.0000
40 URBAN CORE	810229	12	7	11	6	.0322	.0265	.1070	.0809
40 URBAN CORE	810229	12	7	11	7	.0016	.0013	.0000	.0000
40 URBAN CORE	810229	12	7	11	10	.0003	.0002	.0000	.0000
40 URBAN CORE	810229	12	7	11	11	.0004	.0003	.0000	.0000
40 URBAN CORE	810229	12	7	11	12	.0767	.0632	.1858	.1404
40 URBAN CORE	810229	12	7	11	14	.0033	.0028	.0000	.0000
40 URBAN CORE	810229	12	7	11	16	.0001	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	11	18	.0118	.0098	.0000	.0000
40 URBAN CORE	810229	12	7	11	19	.1705	.1404	.5489	.4150
40 URBAN CORE	810229	12	7	11	20	.0005	.0004	.0000	.0000
40 URBAN CORE	810229	12	7	11	21	.0630	.0518	.1492	.1128
40 URBAN CORE	810229	12	7	11	22	.0146	.0120	.0000	.0000
40 URBAN CORE	810229	12	7	11	24	.0021	.0018	.0000	.0000
40 URBAN CORE	810229	12	7	11	26	.0288	.0237	.0310	.0234
40 URBAN CORE	810229	12	7	11	28	.0043	.0035	.0000	.0000
40 URBAN CORE	810229	12	7	12	1	.0000	.0000	2.2289	3.4552
40 URBAN CORE	810229	12	7	12	2	.0000	.0000	.0062	.0101
40 URBAN CORE	810229	12	7	12	5	.0000	.0000	.0012	.0020
40 URBAN CORE	810229	12	7	12	6	.0000	.0000	.0080	.0130
40 URBAN CORE	810229	12	7	12	8	.0000	.0000	.0646	.1045
40 URBAN CORE	810229	12	7	12	10	.0000	.0000	.0107	.0173
40 URBAN CORE	810229	12	7	12	11	.0000	.0000	.0013	.0022
40 URBAN CORE	810229	12	7	12	12	.0000	.0000	.0410	.0663
40 URBAN CORE	810229	12	7	12	14	.0000	.0000	.0089	.0144
40 URBAN CORE	810229	12	7	12	15	.0000	.0000	.0012	.0019
40 URBAN CORE	810229	12	7	12	16	.0000	.0000	.0049	.0079
40 URBAN CORE	810229	12	7	12	19	.0000	.0000	.2630	.4254
40 URBAN CORE	810229	12	7	12	21	.0000	.0000	.0029	.0047
40 URBAN CORE	810229	12	7	12	27	.0000	.0000	.3923	.6345
40 URBAN CORE	810229	12	7	12	28	.0000	.0000	.1181	.1911
40 URBAN CORE	810229	12	7	13	1	.0763	.4535	.0000	.0000
40 URBAN CORE	810229	12	7	13	2	.0005	.0030	.0000	.0000
40 URBAN CORE	810229	12	7	13	6	.0047	.0290	.0000	.0000
40 URBAN CORE	810229	12	7	13	8	.0014	.0087	.0000	.0000
40 URBAN CORE	810229	12	7	13	10	.0016	.0098	.0000	.0000
40 URBAN CORE	810229	12	7	13	11	.0002	.0013	.0000	.0000
40 URBAN CORE	810229	12	7	13	12	.0244	.1495	.0000	.0000
40 URBAN CORE	810229	12	7	13	14	.0007	.0043	.0000	.0000
40 URBAN CORE	810229	12	7	13	15	.0066	.0407	.0000	.0000

TABLE C-8 (CONTINUED)

40 URBAN CORE	810229	12	7	13	16	.0005	.0033	.0000	.0000
40 URBAN CORE	810229	12	7	13	18	.0006	.0036	.0000	.0000
40 URBAN CORE	810229	12	7	13	19	.0019	.0117	.0000	.0000
40 URBAN CORE	810229	12	7	13	21	.0038	.0234	.0000	.0000
40 URBAN CORE	810229	12	7	13	24	.0002	.0009	.0000	.0000
40 URBAN CORE	810229	12	7	13	25	.0000	.0003	.0000	.0000
40 URBAN CORE	810229	12	7	13	26	.0009	.0056	.0000	.0000
40 URBAN CORE	810229	12	7	13	28	.0010	.0059	.0000	.0000
40 URBAN CORE	810229	12	7	14	1	.0605	.2501	.0000	.0000
40 URBAN CORE	810229	12	7	14	2	.0004	.0017	.0000	.0000
40 URBAN CORE	810229	12	7	14	5	.0001	.0004	.0000	.0000
40 URBAN CORE	810229	12	7	14	6	.0008	.0034	.0000	.0000
40 URBAN CORE	810229	12	7	14	8	.0003	.0011	.0000	.0000
40 URBAN CORE	810229	12	7	14	10	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	14	11	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	14	12	.0013	.0054	.0000	.0000
40 URBAN CORE	810229	12	7	14	14	.0064	.0271	.0000	.0000
40 URBAN CORE	810229	12	7	14	15	.0105	.0447	.0000	.0000
40 URBAN CORE	810229	12	7	14	18	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	14	19	.0025	.0108	.0000	.0000
40 URBAN CORE	810229	12	7	14	21	.0006	.0026	.0000	.0000
40 URBAN CORE	810229	12	7	14	24	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	14	25	.0000	.0001	.0000	.0000
40 URBAN CORE	810229	12	7	14	26	.0004	.0015	.0000	.0000
40 URBAN CORE	810229	12	7	14	27	.0064	.0271	.0000	.0000
40 URBAN CORE	810229	12	7	14	28	.0019	.0080	.0000	.0000
40 URBAN CORE	810229	12	7	14	29	.0034	.0147	.0000	.0000
40 URBAN CORE	810229	12	7	16	1	7.4027	2.9194	13.8741	11.3240
40 URBAN CORE	810229	12	7	16	6	.3701	.1766	2.7748	2.4354
40 URBAN CORE	810229	12	7	16	14	.1481	.0707	.2775	.2435
40 URBAN CORE	810229	12	7	16	19	4.4416	2.1197	.4162	.3653
40 URBAN CORE	810229	12	7	16	21	.1851	.0883	1.3874	1.2177
40 URBAN CORE	810229	12	7	16	27	.5922	.2826	2.6361	2.3136
40 URBAN CORE	810229	12	7	17	1	8.2208	12.2522	.0000	.0000
40 URBAN CORE	810229	12	7	17	12	.0822	.1280	.0000	.0000
40 URBAN CORE	810229	12	7	17	19	4.1104	6.3977	.0000	.0000
40 URBAN CORE	810229	12	7	17	27	.3288	.5118	.0000	.0000
40 URBAN CORE	810229	12	7	19	1	-.1872	11.0124	.0000	.0000
40 URBAN CORE	810229	12	7	19	19	-.1872	11.0124	.0000	.0000
3 BACKGROUND	810229	12	7		12				
30 BACKGROUND	810229	12	7		1	28.0000	3.0000	37.0000	4.0000
30 BACKGROUND	810229	12	7		2	.0700	.0550	.7390	.1710
30 BACKGROUND	810229	12	7		3	.0140	.0060	.0010	.0040
30 BACKGROUND	810229	12	7		4	.1460	.0180	.0860	.0160

TABLE C-8 (CONTINUED)

30 BACKGROUND	810229	12	7	5	.1640	.0100	.0640	.0050
30 BACKGROUND	810229	12	7	6	.1280	.0080	3.8050	.4440
30 BACKGROUND	810229	12	7	7	.0010	.0020	.0010	.0020
30 BACKGROUND	810229	12	7	8	.0100	.0070	.0140	.0100
30 BACKGROUND	810229	12	7	9	.0080	.0030	.0010	.0030
30 BACKGROUND	810229	12	7	10	.0100	.0050	.0025	.0050
30 BACKGROUND	810229	12	7	11	.0270	.0030	.0040	.0020
30 BACKGROUND	810229	12	7	12	.1200	.0080	.6920	.0440
30 BACKGROUND	810229	12	7	13	.0015	.0030	.0090	.0030
30 BACKGROUND	810229	12	7	14	.1860	.0100	.2150	.0320
30 BACKGROUND	810229	12	7	15	.0220	.0040	.0180	.0040
30 BACKGROUND	810229	12	7	16	.0030	.0020	.0010	.0020
30 BACKGROUND	810229	12	7	17	.1030	.0180	.0200	.0220
30 BACKGROUND	810229	12	7	18	.8940	.0470	.2130	.0170
30 BACKGROUND	810229	12	7	19	14.7800	.7650	.8520	.7830
30 BACKGROUND	810229	12	7	20	.0080	.0030	.0010	.0030
30 BACKGROUND	810229	12	7	21	.1890	.0270	4.0000	.9140
30 BACKGROUND	810229	12	7	22	.0240	.0030	.0030	.0030
30 BACKGROUND	810229	12	7	23	.0030	.0020	.0060	.0020
30 BACKGROUND	810229	12	7	24	.0080	.0160	.0970	.0170
30 BACKGROUND	810229	12	7	25	.0030	.0090	.0035	.0070
30 BACKGROUND	810229	12	7	26	.0380	.0030	.0160	.0030
40 BACKGROUND	810229	12	7	1 1	-.3337	.3463	20.2530	5.8613
40 BACKGROUND	810229	12	7	1 2	-.0022	.0024	.1114	.0434
40 BACKGROUND	810229	12	7	1 6	-.0310	.0341	1.0329	.4020
40 BACKGROUND	810229	12	7	1 11	-.0001	.0001	.0018	.0007
40 BACKGROUND	810229	12	7	1 12	-.0028	.0030	.0972	.0378
40 BACKGROUND	810229	12	7	1 14	-.0007	.0007	.0243	.0095
40 BACKGROUND	810229	12	7	1 15	-.0001	.0001	.0043	.0017
40 BACKGROUND	810229	12	7	1 18	.0000	.0001	.0041	.0016
40 BACKGROUND	810229	12	7	1 19	-.0015	.0016	.0547	.0213
40 BACKGROUND	810229	12	7	1 21	-.0080	.0088	.4861	.1892
40 BACKGROUND	810229	12	7	1 23	-.0001	.0001	.0028	.0011
40 BACKGROUND	810229	12	7	1 24	-.0005	.0005	.0180	.0070
40 BACKGROUND	810229	12	7	1 26	-.0001	.0001	.0018	.0007
40 BACKGROUND	810229	12	7	1 30	.0000	.0000	.0004	.0002
40 BACKGROUND	810229	12	7	2 1	.2138	.6555	6.1296	1.3633
40 BACKGROUND	810229	12	7	2 2	.0189	.0599	.4039	.1370
40 BACKGROUND	810229	12	7	2 5	.0000	.0001	.0005	.0002
40 BACKGROUND	810229	12	7	2 6	.0052	.0165	.1839	.0624
40 BACKGROUND	810229	12	7	2 10	.0001	.0003	.0000	.0000
40 BACKGROUND	810229	12	7	2 11	.0001	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	2 12	.0128	.0407	.3512	.1191
40 BACKGROUND	810229	12	7	2 14	.0022	.0070	.0000	.0000
40 BACKGROUND	810229	12	7	2 15	.0003	.0008	.0061	.0021
40 BACKGROUND	810229	12	7	2 16	.0000	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	2 18	.0008	.0025	.0000	.0000
40 BACKGROUND	810229	12	7	2 19	.0024	.0075	.0000	.0000

TABLE C-8 (CONTINUED)

40 BACKGROUND	810229	12	7	2	21	.0477	.1512	1.7408	.5905
40 BACKGROUND	810229	12	7	2	24	.0014	.0043	.0619	.0210
40 BACKGROUND	810229	12	7	2	25	.0000	.0002	.0017	.0006
40 BACKGROUND	810229	12	7	2	26	.0002	.0007	.0000	.0000
40 BACKGROUND	810229	12	7	2	27	.0292	.0925	.2997	.1017
40 BACKGROUND	810229	12	7	2	28	.0027	.0085	.1073	.0364
40 BACKGROUND	810229	12	7	2	29	.0000	.0000	.0012	.0004
40 BACKGROUND	810229	12	7	3	1	-.1872	.0933	-.0240	.0311
40 BACKGROUND	810229	12	7	3	6	-.0019	.0011	-.0002	.0003
40 BACKGROUND	810229	12	7	3	8	-.1029	.0588	-.0132	.0179
40 BACKGROUND	810229	12	7	3	14	-.0019	.0011	-.0002	.0003
40 BACKGROUND	810229	12	7	3	19	-.0168	.0096	-.0022	.0029
40 BACKGROUND	810229	12	7	3	28	-.0580	.0332	-.0074	.0101
40 BACKGROUND	810229	12	7	5	1	12.5377	7.3249	1.7490	4.8223
40 BACKGROUND	810229	12	7	5	2	.0150	.0098	.0021	.0060
40 BACKGROUND	810229	12	7	5	6	.0213	.0139	.0030	.0085
40 BACKGROUND	810229	12	7	5	11	.0030	.0020	.0004	.0012
40 BACKGROUND	810229	12	7	5	12	.0138	.0090	.0019	.0055
40 BACKGROUND	810229	12	7	5	14	.0055	.0036	.0008	.0022
40 BACKGROUND	810229	12	7	5	15	.0019	.0012	.0003	.0007
40 BACKGROUND	810229	12	7	5	16	.0019	.0012	.0003	.0007
40 BACKGROUND	810229	12	7	5	19	6.2689	4.0875	.8745	2.4949
40 BACKGROUND	810229	12	7	5	21	.0639	.0417	.0089	.0254
40 BACKGROUND	810229	12	7	5	26	.0100	.0065	.0014	.0040
40 BACKGROUND	810229	12	7	5	27	4.8897	3.1883	.6821	1.9461
40 BACKGROUND	810229	12	7	6	1	1.8886	.6088	.5401	.1058
40 BACKGROUND	810229	12	7	6	2	.0008	.0003	.0002	.0001
40 BACKGROUND	810229	12	7	6	5	.1549	.0644	.0443	.0142
40 BACKGROUND	810229	12	7	6	8	.1020	.0424	.0292	.0094
40 BACKGROUND	810229	12	7	6	11	.0001	.0000	.0000	.0000
40 BACKGROUND	810229	12	7	6	12	.0047	.0020	.0014	.0004
40 BACKGROUND	810229	12	7	6	18	.3985	.1657	.1140	.0366
40 BACKGROUND	810229	12	7	6	19	.0040	.0016	.0011	.0004
40 BACKGROUND	810229	12	7	6	21	.0014	.0006	.0004	.0001
40 BACKGROUND	810229	12	7	6	26	.0004	.0002	.0001	.0000
40 BACKGROUND	810229	12	7	6	27	1.0293	.4280	.2943	.0946
40 BACKGROUND	810229	12	7	9	1	1.5719	3.7865	.0000	.0000
40 BACKGROUND	810229	12	7	9	2	.0049	.0122	.0000	.0000
40 BACKGROUND	810229	12	7	9	5	.0004	.0010	.0000	.0000
40 BACKGROUND	810229	12	7	9	6	.0079	.0196	.0000	.0000
40 BACKGROUND	810229	12	7	9	8	.0189	.0471	.0000	.0000
40 BACKGROUND	810229	12	7	9	11	.0027	.0067	.0000	.0000

TABLE C-8 (CONTINUED)

40 BACKGROUND	810229	12	7	9	12	.0019	.0047	.0000	.0000
40 BACKGROUND	810229	12	7	9	14	.0003	.0007	.0000	.0000
40 BACKGROUND	810229	12	7	9	15	.0002	.0005	.0000	.0000
40 BACKGROUND	810229	12	7	9	16	.0001	.0004	.0000	.0000
40 BACKGROUND	810229	12	7	9	18	.0085	.0212	.0000	.0000
40 BACKGROUND	810229	12	7	9	19	.2075	.5178	.0000	.0000
40 BACKGROUND	810229	12	7	9	21	.0042	.0106	.0000	.0000
40 BACKGROUND	810229	12	7	9	25	.0001	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	9	26	.0005	.0011	.0000	.0000
40 BACKGROUND	810229	12	7	9	27	.5628	1.4043	.0000	.0000
40 BACKGROUND	810229	12	7	9	28	.0050	.0126	.0000	.0000
40 BACKGROUND	810229	12	7	9	29	.0157	.0392	.0000	.0000
40 BACKGROUND	810229	12	7	10	1	-.7351	.7328	.0000	.0000
40 BACKGROUND	810229	12	7	10	6	-.0368	.0389	.0000	.0000
40 BACKGROUND	810229	12	7	10	19	-.3455	.3654	.0000	.0000
40 BACKGROUND	810229	12	7	10	27	-.0882	.0933	.0000	.0000
40 BACKGROUND	810229	12	7	11	1	1.0883	.9506	1.3968	.8400
40 BACKGROUND	810229	12	7	11	2	.0048	.0045	.0000	.0000
40 BACKGROUND	810229	12	7	11	4	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	11	6	.0198	.0185	.0330	.0220
40 BACKGROUND	810229	12	7	11	7	.0010	.0009	.0000	.0000
40 BACKGROUND	810229	12	7	11	10	.0002	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	11	11	.0002	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	11	12	.0472	.0441	.0573	.0383
40 BACKGROUND	810229	12	7	11	14	.0021	.0019	.0000	.0000
40 BACKGROUND	810229	12	7	11	16	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	11	18	.0073	.0068	.0000	.0000
40 BACKGROUND	810229	12	7	11	19	.1048	.0979	.1692	.1131
40 BACKGROUND	810229	12	7	11	20	.0003	.0003	.0000	.0000
40 BACKGROUND	810229	12	7	11	21	.0387	.0362	.0460	.0307
40 BACKGROUND	810229	12	7	11	22	.0090	.0084	.0000	.0000
40 BACKGROUND	810229	12	7	11	24	.0013	.0012	.0000	.0000
40 BACKGROUND	810229	12	7	11	26	.0177	.0165	.0095	.0064
40 BACKGROUND	810229	12	7	11	28	.0026	.0025	.0000	.0000
40 BACKGROUND	810229	12	7	12	1	.0000	.0000	.0531	.5375
40 BACKGROUND	810229	12	7	12	2	.0000	.0000	.0001	.0016
40 BACKGROUND	810229	12	7	12	5	.0000	.0000	.0000	.0003
40 BACKGROUND	810229	12	7	12	6	.0000	.0000	.0002	.0020
40 BACKGROUND	810229	12	7	12	8	.0000	.0000	.0015	.0161
40 BACKGROUND	810229	12	7	12	10	.0000	.0000	.0003	.0027
40 BACKGROUND	810229	12	7	12	11	.0000	.0000	.0000	.0003
40 BACKGROUND	810229	12	7	12	12	.0000	.0000	.0010	.0102
40 BACKGROUND	810229	12	7	12	14	.0000	.0000	.0002	.0022
40 BACKGROUND	810229	12	7	12	15	.0000	.0000	.0000	.0003
40 BACKGROUND	810229	12	7	12	16	.0000	.0000	.0001	.0012
40 BACKGROUND	810229	12	7	12	19	.0000	.0000	.0063	.0654

TABLE C-8 (CONTINUED)

40 BACKGROUND	810229	12	7	12	21	.0000	.0000	.0001	.0007
40 BACKGROUND	810229	12	7	12	27	.0000	.0000	.0093	.0975
40 BACKGROUND	810229	12	7	12	28	.0000	.0000	.0028	.0294
40 BACKGROUND	810229	12	7	13	1	-.0525	.1141	.0000	.0000
40 BACKGROUND	810229	12	7	13	2	-.0003	.0008	.0000	.0000
40 BACKGROUND	810229	12	7	13	6	-.0033	.0073	.0000	.0000
40 BACKGROUND	810229	12	7	13	8	-.0010	.0022	.0000	.0000
40 BACKGROUND	810229	12	7	13	10	-.0011	.0025	.0000	.0000
40 BACKGROUND	810229	12	7	13	11	-.0001	.0003	.0000	.0000
40 BACKGROUND	810229	12	7	13	12	-.0168	.0378	.0000	.0000
40 BACKGROUND	810229	12	7	13	14	-.0005	.0011	.0000	.0000
40 BACKGROUND	810229	12	7	13	15	-.0046	.0103	.0000	.0000
40 BACKGROUND	810229	12	7	13	16	-.0004	.0008	.0000	.0000
40 BACKGROUND	810229	12	7	13	18	-.0004	.0009	.0000	.0000
40 BACKGROUND	810229	12	7	13	19	-.0013	.0030	.0000	.0000
40 BACKGROUND	810229	12	7	13	21	-.0026	.0059	.0000	.0000
40 BACKGROUND	810229	12	7	13	24	-.0001	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	13	25	.0000	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	13	26	-.0006	.0014	.0000	.0000
40 BACKGROUND	810229	12	7	13	28	-.0007	.0015	.0000	.0000
40 BACKGROUND	810229	12	7	14	1	.1465	.1368	.0000	.0000
40 BACKGROUND	810229	12	7	14	2	.0009	.0009	.0000	.0000
40 BACKGROUND	810229	12	7	14	5	.0002	.0002	.0000	.0000
40 BACKGROUND	810229	12	7	14	6	.0019	.0019	.0000	.0000
40 BACKGROUND	810229	12	7	14	8	.0006	.0006	.0000	.0000
40 BACKGROUND	810229	12	7	14	10	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	14	11	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	14	12	.0031	.0031	.0000	.0000
40 BACKGROUND	810229	12	7	14	14	.0154	.0153	.0000	.0000
40 BACKGROUND	810229	12	7	14	15	.0254	.0252	.0000	.0000
40 BACKGROUND	810229	12	7	14	18	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	14	19	.0062	.0061	.0000	.0000
40 BACKGROUND	810229	12	7	14	21	.0015	.0014	.0000	.0000
40 BACKGROUND	810229	12	7	14	24	.0001	.0001	.0000	.0000
40 BACKGROUND	810229	12	7	14	25	.0000	.0000	.0000	.0000
40 BACKGROUND	810229	12	7	14	26	.0008	.0008	.0000	.0000
40 BACKGROUND	810229	12	7	14	27	.0154	.0153	.0000	.0000
40 BACKGROUND	810229	12	7	14	28	.0045	.0045	.0000	.0000
40 BACKGROUND	810229	12	7	14	29	.0084	.0083	.0000	.0000
40 BACKGROUND	810229	12	7	16	1	2.8841	1.1658	6.9544	2.6936
40 BACKGROUND	810229	12	7	16	6	.1442	.0701	1.3909	.6552
40 BACKGROUND	810229	12	7	16	14	.0577	.0280	.1391	.0655
40 BACKGROUND	810229	12	7	16	19	1.7305	.8408	.2086	.0983
40 BACKGROUND	810229	12	7	16	21	.0721	.0350	.6954	.3276

TABLE C-8 (CONTINUED)

40 BACKGROUND	810229 12	7 16 27	.2307	.1121	1.3213	.6224
40 BACKGROUND	810229 12	7 17 1	4.5964	4.5043	.0000	.0000
40 BACKGROUND	810229 12	7 17 12	.0460	.0478	.0000	.0000
40 BACKGROUND	810229 12	7 17 19	2.2982	2.3915	.0000	.0000
40 BACKGROUND	810229 12	7 17 27	.1839	.1913	.0000	.0000
40 BACKGROUND	810229 12	7 19 1	4.0254	4.4807	.0000	.0000
40 BACKGROUND	810229 12	7 19 19	4.0254	4.4807	.0000	.0000

APPENDIX D

STATISTICAL APPROACH FOR SOURCE APPORTIONMENT

This appendix presents a discussion of the statistical methods used in the source apportionment software documented herein. First, the source apportionment problem is formulated in mathematical terms. This involves primarily stating the mass balance equations used in source apportionment.

Subsequently a discussion of the statistical methods used in the software documented herein is presented. The basic approach used is regression analysis. However, several additional features are available to handle specific aspects of the problem.

While Section 2 discusses source apportionment strictly from a user's viewpoint, this appendix discusses the mathematics, with references to papers which provide further detail. For the convenience of the reader, Section 2 and this appendix have both been made as nearly self-contained as is feasible. As a result, some overlap exists between the two discussions.

Mathematical Formulation of the Problem

The standard equation used in CMB analysis is as follows:

$$C_i = \sum_{j=1}^m F_{ij} S_j \quad (1)$$

where

C_i is the ambient particulate concentration of species i ,

F_{ij} is the fraction of the particulate matter emitted from source j comprised of species i ,

S_j is the ambient particulate concentration resulting from source j ,
and

m is the number of sources.

All inputs pertain to the size fraction being considered.

The C_i values are obtained through chemical analysis of ambient particulate samples. The F_{ij} values are obtained through direct source characterization or by indirect methods, such as sampling upwind and downwind of a source. The C_i and F_{ij} values are required inputs. Depending on the type of statistical analysis performed, the standard errors of the C_i and F_{ij} values may also be included. The "standard error" of a quantity is the standard deviation of its random error. The values of S_j represent the contributions of the different sources to the ambient particulate concentration, and, as such, are the unknown values.

If multiple particulate samples have been collected for a specific set of conditions, averaging can be performed to produce a single concentration for each species. Subsequently, a single CMB analysis can be performed using the averaged concentrations. An alternative is to perform a separate CMB analysis for each particulate sample and then average the CMB results for each source. In this case, however, the error present in the source signature (F_{ij}) matrix would be common to all periods. Thus, the separate CMB analyses would have correlated errors. For this reason, the conventional standard error of the mean would have a low bias (see the discussion of this point in Section 2).

At the option of the user, an intercept term S_o can be added to the standard equation:

$$C_i = S_o + \sum_{j=1}^m F_{ij} S_j \quad (2)$$

The intercept represents a part of the particulate concentration not accounted for by the m sources considered. Thus, the intercept should be zero within random error unless there is a significant source which has not been considered or large data errors exist. The intercept provides a check on the closure of the mass balance equations. If the regression is performed with no intercept, all variances are computed about zero, not about the mean values.

An additional equation can also be employed:

$$C_T = S_o + \sum_{j=1}^m S_j \quad (3)$$

where C_T is the measured aerosol mass concentration for the size fraction being considered. This equation simply states that the sum of the intercept and the particulate concentrations attributable to the m sources equals the ambient aerosol mass concentration. The intercept here is again the particulate concentration not explainable by any of the sources considered. Thus, as before, the intercept should be near zero unless there is a significant omitted source or large data errors.

Statistical Approaches

Regression analysis is the basic statistical approach which has been employed in the program documented herein (Cooper et al., 1979; Kowalczyk et al., 1978). Regression analysis is very versatile in that it can be modified in various ways to handle the different conditions which can arise. Several such properties of the CMB problem, which require special features not provided by ordinary multiple regression analysis, are discussed below.

First, in the regression analysis, the C_i and C_T are the values of the dependent variable, and it is known that these values have different error variances. To account for this fact, weighted least squares should be used.

This approach differs from ordinary multiple regression in that the most accurate data are weighted most heavily in developing the regression equation. In ordinary multiple regression, all data are weighted equally. In weighted regression, the values of S_o and S_j , $j=1$ to m , are chosen so as to minimize the sum of squares SS:

$$SS = \sum_{i=1}^n \frac{(\hat{C}_i - C_i)^2}{s_{C_i}^2} + \frac{(\hat{C}_T - C_T)^2}{s_{C_T}^2} \quad (4)$$

where

$\hat{C}_i$ and $\hat{C}_T$ are concentrations predicted by equations (2) and (3), respectively,

C_i and C_T are the corresponding measured concentrations,

$s_{C_i}^2$ and $s_{C_T}^2$ are the error variances of C_i and C_T , respectively, and

n is the number of chemical species being considered.

Second, in ordinary multiple regression analysis, it is assumed that the predictor variables have no error. In the CMB analysis, however, the values of the predictor variables (F_{ij}) have random errors. Approaches to account for these errors in the CMB analysis have been described by Watson (1979). In one approach, the C_i and F_{ij} values are all weighted according to their uncertainties in achieving a maximum-likelihood solution of the mass balance equations (Eq. 1). The approach requires an iterative solution, however, which sometimes fails to achieve convergence. A simpler method uses "effective variances" to account for the errors in the F_{ij} . In this approach, the variance of the total error in each mass balance equation, including the error of C_i and the errors in the terms involving the F_{ij} , is taken into account. The resulting effective variance for the i^{th} equation is

$$s_{EV_i}^2 = s_{C_i}^2 + \sum_{j=1}^m S_j^2 s_{F_{ij}}^2 \quad (5)$$

A weighted least squares analysis is performed, and effective variances are used in place of error variances of ambient concentration measurement error variances.

In the mass balance equation involving aerosol mass concentration (Eq. 3), the coefficients of the S_j are all unity and have zero error variances. Thus, the effective variance of this equation is simply the error variance of C_T . Using effective variances, then, increases the error variances associated with all other equations (Eq. 2) relative to the error variance for the equation involving aerosol mass concentration (Eq. 3). Thus, the use of effective variances increases the relative weight given to the aerosol mass equation (Eq. 3). Use of effective variances will not always improve the agreement between the measured and predicted aerosol mass concentrations, however. This is because of the complex shifting of the relative weights given to all the equations.

Since the effective-variance calculation involves the unknown S_j values, an initial solution estimate is required. Thus, an iterative approach can be used; the initial estimate at each stage is the solution from the preceding iteration.

Another important aspect of the CMB approach involves the difficulty in estimating the separate particulate contributions of sources whose aerosols have similar chemical compositions. If the compositions were identical, it would be impossible to differentiate between the aerosols from the two sources. If the compositions were very similar, differentiation would be possible but difficult to accomplish accurately. The problem is referred to in statistical terms as "multicollinearity." Stated more generally, multicollinearity exists when any source signature is very nearly a linear combination of any subset of the other signatures. In this case, it is difficult to distinguish among the aerosols emanating from the sources with nearly linearly dependent signatures. Multicollinearity can cause large random errors if conventional weighted least squares with or

without effective variances is used. Negative values with large magnitudes can result from these errors.

Ridge regression is an approach for handling problems with multicollinearity. A brief summary of the properties of ridge regression which are essential to the discussion here is presented below. Ridge regression is discussed further by Vinod (1978), Hoerl and Kennard (1970a, b), Marquardt (1970), Swindel (1974), Marquart and Snee (1975), and Obenchain (1977). The use of ridge regression in source apportionment is discussed by Williamson, Balfour, and Schmidt (1982).

In ordinary regression analysis,

$$B = (x'x)^{-1} x'y \quad (6)$$

where

B is the vector of regression coefficients - in CMB analysis, the intercept S_0 and the S_j ,
 x is the design matrix, here the source signature matrix,
 y is the vector of values of the dependent variable, here the species and total particulate concentrations,
 the prime indicates matrix transposition,
 and the superscript $^{-1}$ indicates matrix inversion.

In ridge regression, a parameter k is introduced:

$$B(k) = (x'x + kI)^{-1} x'y \quad (7)$$

where

B(k) is the ridge solution corresponding to the parameter k, and
 I is the identity matrix.

Notice that if $k = 0$, the ridge solution becomes the ordinary regression solution.

The usual practice is to standardize $x'x$ and $x'y$ to contain correlation coefficients. The B values obtained from Eq. 6 are then called standardized coefficients. The solution in terms of the original data units is obtained by an inverse transformation. The diagonal elements of $x'x$, then, are all one. A k value of, for example, 0.1 represents a 10 percent perturbation of the diagonal elements. If k is positive, a bias is introduced into the regression coefficients; the conventional regression solution is unbiased. However, the error variances of the coefficients, if inflated due to multicollinearities, often decrease rapidly as k increases. Thus, a much improved solution can be achieved when, by introducing a small bias, a large reduction of the random errors is accomplished.

Variance-inflation factors (Belsley et al., 1980) are convenient measures of the effect of multicollinearity in a given problem. The variance-inflation factor of a given regression coefficient (S_j) can be interpreted as the ratio of its error variance to the error variance it would have had if the predictor variables had been uncorrelated.

The covariance matrix C of the standardized regression coefficients is

$$C = (x'x)^{-1} \sigma^2 \quad (8)$$

where σ^2 is the error variance of the dependent variable. The error variances of the regression coefficients are the diagonal elements of C. The error variances which would have been obtained if the predictor variables were uncorrelated are obtained by setting the off-diagonal elements of $x'x$ equal to zero and employing Eq. 8. The variance inflation factors, then, are the ratios of the actual error variances to those obtained assuming uncorrelated predictor variables. The variance inflation factors apply either to the standardized or unstandardized regression coefficients, since the scale factors cancel in taking the ratio.

If multicollinearities are present, the regression coefficients are usually extremely sensitive to k for small values of k . However, as k increases, the coefficients stabilize. Hoerl and Kennard (1970a, b) recommend selecting a value of k in the stable region within which moderate changes in k do not affect the coefficients significantly.

A diversity of automatic statistical approaches for selecting k have been discussed in the literature, e.g., by Dempster et al. (1977), and Wichern and Churchill (1978). In the program documented herein, the user has the option of displaying the solutions for a set of values of k or letting the program select k . The automatic method is based on both statistical and physical criteria. The motivation for choosing the particular criteria used is as follows. Typically, when serious multicollinearities are present, in the weighted least squares solution, one S_j value in a collinear set will be excessively large and another will be negative with large magnitude. That is, one S_j value will blow up on the positive side and another will blow up on the negative side. Simply setting the negative values equal to zero, therefore, would solve only half of the problem.

As k increases, the negative values usually approach zero, and some or all of them may become positive. Thus, one criterion is to select k so as to minimize the magnitudes of the negative S_j values.

Another criterion is to optimize the agreement between the observed and calculated aerosol concentration for the size fraction being considered. This criterion involves the complete set of S_j values and has a reasonable physical basis. To address both criteria k is selected so as to minimize the following:

$$(\hat{C}_T - C_T)^2 + W \sum_{S_j < 0} S_j^2 \quad (9)$$

where W is a user-specified weighting factor. Increasing W increases the relative importance of avoiding negative values with significant magnitudes. Decreasing W increases the relative importance of achieving agreement between the measured and calculated aerosol mass concentrations. The sum of squares of the negative S_j values is zero if there are no negatives.

While this is obviously only one of many possible schemes for selecting k , it is based on reasonable physical and statistical criteria. Nevertheless, neither this nor any automatic scheme can guarantee selection of the optimal value of k . However, the suggested scheme tends to select values of k in the stable region. Thus, slight deviation from the optimal k should not introduce significant errors in the solution.

Weighted regression, effective-variance calculations, and ridge regression all offer enhancements to the ordinary multiple regression approach to the CMB problem. Fortunately, these three features can be used simultaneously or in various combinations. In weighted regression, a transformation is first made to stabilize the error variance of the dependent variable (Draper and Smith, 1966). This transformation can be made using the original error variances of the dependent variable or the effective variances. Subsequently, the regression analysis is performed using the transformed variables; this can be accomplished using either ordinary regression or ridge regression. Finally, the necessary inverse transformation is performed to obtain the solution in the original data units.

The simultaneous use of the three features mentioned above requires certain minor changes to the procedures. For example, weighted ridge regression with an intercept is most easily carried out if $x'x$ and $x'y$ are normalized but not centered. Thus, $x'x$ and $x'y$ do not contain correlation coefficients, as in conventional ridge regression practices discussed above. However, the diagonal elements of $x'x$ are unity, as in the conventional case. Thus, as before, a k value of 0.1 represents a 10 percent perturbation of the diagonal elements. This and other minor procedural changes do not impact the interpretability of the results.

In the discussion above, the expression for the covariance matrix of the standardized regression coefficients is given in Eq. 8. The quantity σ^2 is the error variance of the dependent variable; a common error variance applies after the transformation to stabilize the variance has been performed.

The quantity σ^2 is estimated by s^2 , the conventional standard error:

$$s^2 = \frac{\sum_{i=1}^{n+1} (\hat{Y}_i - Y_i)^2}{n+1 - L} \quad (10)$$

where

Y_i is the i^{th} value of the dependent variable, i.e., Y_i is the measured concentration of the i^{th} species, $1 \leq i \leq n$, and Y_{n+1} is the measured aerosol mass concentration after the transformation to standardize the variance,

$\hat{Y}_i$ is the i^{th} predicted value,

n is the number of species as before, and

L is the number of regression coefficients estimated - $m+1$ if the intercept is included and m if not.

The standard errors of the S_j values, then, are rescaled to the original data units in exactly the same manner as are the S_j values.

Thus, the input standard errors of the concentration and source signature data are used only for weighting purposes. Neither the S_j values nor their standard errors are directly proportional to the input standard errors. This is advantageous, since accurate estimates of the standard errors of the source signatures are not now available. The basic error measure s^2 is derived directly from the differences between observed and predicted concentrations.

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16. ABSTRACT In recent years there has been increasing interest in source apportionment of ambient aerosol concentrations through chemical mass balance (CMB) analysis. This report discusses CMB analysis through weighted least squares with options to include effective variance and ridge regression features. Effective variances are refined estimates of the weights employed in weighted least squares. This report documents an interactive FORTRAN computer program which performs aerosol source apportionment through the analysis methods discussed above. The original version of the program, which performed weighted least squares with the effective variance option, was developed at the Oregon Graduate Center based on the Doctoral Dissertation of Dr. John Watson. In the current version, a ridge regression feature was added, along with various modifications intended to enhance the ease of use of the program.		
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