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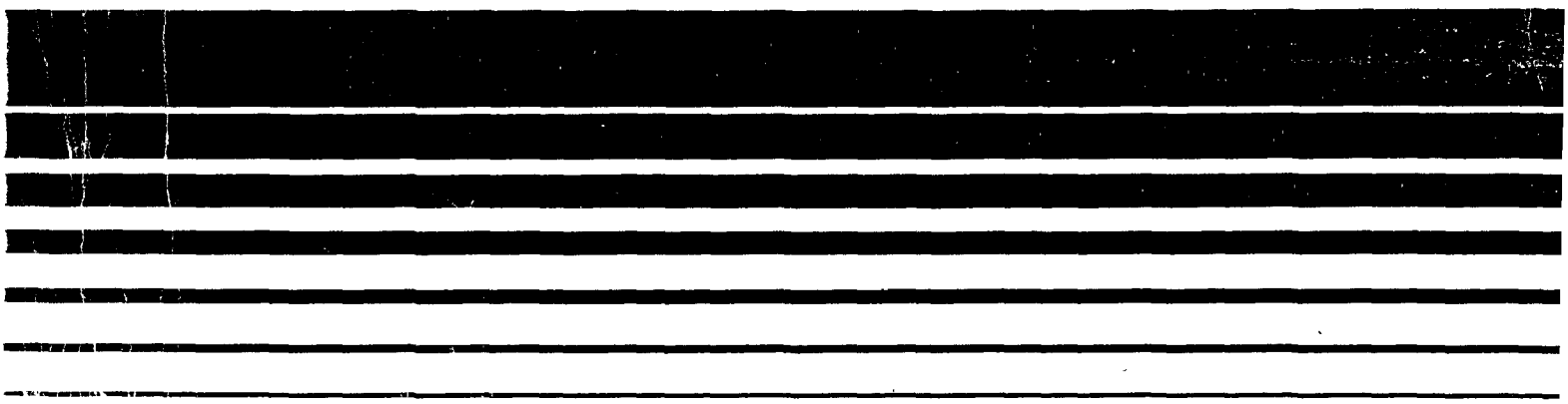
Chemical Mass Balance Receptor Model Diagnostics



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Chemical Mass Balance Receptor Model Diagnostics

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Executive Summary

The purpose of this study is to develop, test, and recommend means for identification of influential species in a Chemical Mass Balance (CMB) model. Influential species are defined as those which have a large effect on the estimated source contributions or its errors. Knowledge of the influential species aids the interpretation of CMB results and can suggest schemes to improve a CMB model. The degree of influence of a species can be defined in two ways. One way is to calculate the effects of deleting it from the model; many standard regression diagnostics are based on this approach. The other way uses diagnostics based on a different approach: CMB estimates of source contributions can be interpreted as a weighted sum of the species concentrations at the receptors. Thus, the influence of each species on a particular source is determined by the amount of weight given to it by the CMB least squares fit. These new measures are called nondeletion diagnostics to distinguish them from the deletion diagnostics.

Extensive testing was carried out on two deletion and two nondeletion diagnostics in order to build an experience base with which to compare them. The testing used sets of artificial data generated by two different source composition matrices. One set had four sources and little multicollinearity, while the second had eight sources and substantial collinearity. The measurement error in the species was taken as 10%; the error in the source matrix was 10, 30, or 50 %. Three simulation runs were carried out for each level of error. The means and standard deviations of the diagnostics were determined for each error scenario and served as a convenient way to summarize the results of the simulations. These results agreed with theoretical arguments which showed that a single influence diagnostic based on a modification of the pseudo-inverse matrix (MPIN) was the best choice. Experience gained in the tests on simulated data showed that the MPIN contains virtually all the information present in both deletion and non-deletion diagnostics. The test results support the following recommendations for interpretation of the MPIN diagnostic. MPIN is normalized such that it takes on values from minus one to one. Species with MPIN absolute values of 1 to 0.5 are associated with influential species. Noninfluential species have MPIN absolute values of 0.3 or less. Species with absolute values between 0.3 and 0.5 are ambiguous, but should generally be considered noninfluential.

Table of contents

1. Introduction

Receptor modeling is being used increasingly as a method to identify the sources and to apportion ambient concentrations of particulate pollutants and to determine the best control strategies. These models estimate the source impacts at a receptor site from the measurements of aerosol properties made at the receptor or sampling site. Receptor models and their application have been reviewed by Cooper and Watson (1980), Gordon (1980), and Hopke (1985). Henry et al (1984) has presented a review of receptor model fundamentals.

Usually a least squares fitting approach is applied to Chemical Mass Balance (CMB) models calculations of the source contributions of particulates (Axetell and Watson, 1987; Pace and Watson, 1987). Written in matrix form, the CMB equation is,

$$C = AS, \qquad (1)$$

where C is the nx1 vector of ambient chemical species concentrations, A is the nxp source composition matrix, and S is the px1 vector of source contributions. When estimating the contributions of sources whose chemical compositions are similar, the least squares solution is mathematically unstable, the so called collinearity problem. Henry (1982) presented some rules that can be used to determine which sources in a CMB model can be estimated to a given accuracy

and which cannot be so estimated. The same work also gives a method that allows one to find estimable linear combinations of sources which by themselves cannot be accurately estimated.

In the previous year's work (Henry and Kim, 1986), collinearity indicators were studied. Eigenvectors corresponding to the smallest eigenvalues were found to be the best indicators of the collinearity. Also, guidelines were prepared for users on how to use eigenvectors to detect the sources contributing to the collinearity. The objective of the current project is to examine several regression diagnostics to identify the influential fitting species and provide the best diagnostic and a guideline for its use.

2. Theoretical background

There are several uses for diagnostic tests which identify the most influential species in a CMB calculation. A CMB result that is found to be very heavily dependent upon species which have very uncertain source composition data will obviously be more suspect than one which is known to depend most heavily upon well known species. If possible, steps should be taken to improve the source composition data for the influential species. Perhaps additional source sampling is needed, or reanalysis of existing source samples by a more sensitive analytical technique.

The best application of these diagnostics is in a

proactive manner by assembling and analyzing a tentative source composition matrix before the study, thereby determining where best to apply the available resources. Perhaps additional sampling of one source to better characterize an influential species is not necessary, but the diagnostics may indicate another species in another source for which it is vital to have improved source composition information.

The diagnostics often confirm our intuition in identifying tracer species as influential species. However, because of the interactions among the sources in a least squares fit, at times our intuition may be fooled and the CMB source contribution estimate may depend crucially on some minor species. These cases are not rare and can only be dealt with properly by diagnostics of the type investigated in this study.

2.1 Basic Approach

There are several established diagnostic tools for identifying influential data points. Specifically, DFBETA, DFBETAS, DFFIT, DFFITS, RSTUDENT, and COVRATIO have been most commonly used as diagnostic tools. These are discussed in detail by Belsley et al (1980) and have been applied to the CMB model by DeCesar et al (1985;1986). All the above diagnostics are single row deletion diagnostics. In other words, they examine how the deletion of a single row

(species) affects the estimated regression coefficients (source contribution estimates), the predicted values (species concentrations), the residuals or the estimated covariance structure of the regression coefficients. A species is judged to be influential by these diagnostics if its removal from the CMB leads to a large relative change in one of the aspects of the model listed above.

In addition to single row deletion diagnostics, several nondeletion diagnostics were studied. These diagnostics give the contribution of a species to the source contribution estimate or its error variance in the full model without deletion.

The original plan of this study was to introduce a composite diagnostic tool which incorporates both modified single row deletion diagnostics and nondeletion diagnostics to give a reliable indicator of those species of special importance to the CMB. Nondeletion diagnostics were developed to supplement single row deletion diagnostics under the assumption that species which are influential when deleted from the model are not necessarily those species that have the most influence on the full model results.

The remainder of this report takes the following form. Two selected deletion diagnostics, with minor modifications to increase their interpretability, are described. Next, two nondeletion diagnostics based on the weighted pseudo-inverse (PIN) matrix are introduced. These four diagnostics are then

shown to be similar to a single diagnostic, the modified PIN matrix (MPIN).

The last sections of the report describe the Monte-Carlo simulation studies carried out to test the new diagnostic. Finally, specific numerical recommendations for interpretation of the diagnostic are given.

2.1.1 Deletion diagnostics

The basis of this diagnostic technique is an analysis of the response of various regression model outputs to controlled perturbations of the model inputs. The deletion of a single species from the CMB is usually taken as the perturbation. In this study, changes in the source contribution estimates (SCEs) and the estimated variance of the SCEs in response to the perturbed regression model are the basis for two new deletion diagnostics closely related to the standard DFBETA diagnostic.

The first deletion diagnostic, SDFBETA, is the fractional change in the SCE if a row (species) is deleted from the CMB source composition matrix. The second diagnostic, SDFSBETA, is the fractional change in the variance of the SCE if a row is removed from the source composition matrix. Because of their normalization, both diagnostics are less than or equal to one in absolute value. The closer the absolute value of the diagnostic is to one, the more influential the species.

2.1.1.1 SDFBETA

The change in the SCEs when the ith row is deleted is expressed as DFBETA.

$$DFBETA_i = S - S(i) = \frac{(A^TA)^{-1}a_i^Te_i}{1 - h_i}, \qquad (2)$$

where S(i) is the SCE estimated with the ith row deleted, a_i is a row vector of A, e_i is a ith residual and $h_i = a_i(A^TA)^{-1}a_i^T$ (note that the A in this equation is the full matrix, including a_i). DFBETA is usually normalized to the standard deviation of the SCE to form DFBETAS (Belsley et al, 1980). Experience gained in the previous year's work showed DFBETAS is unstable to errors. In other words, keeping all else constant, even modest random changes in the errors lead to large changes in DFBETAS. For this reason, this study adopted a different normalization. DFBETA is normalized to the SCE itself,

$$SDFBETA_{ij} = \frac{DFBETA_{ij}}{S_j} = \left[\frac{S_j - S_j(i)}{S_j}\right]_{ij}. \qquad (3)$$

With this normalization SDFBETA is more easily interpreted than DFBETAS. However, SDFBETA is also unstable to errors, like DFBETAS, even if little or no collinearity is present. This instability is caused by the presence of the residual, e_i, in Eq.2. Table A2 - Table A7 in appendix demonstrates this point. Therefore, SDFBETA is not recommended as a

diagnostic tool.

2.1.1.2 SDFSBETA

The change of the estimated variance of the SCE when the ith row is deleted is also of interest to users. This change is calculated in Silvey (1969) and normalized to the variance of the SCEs to form SDFSBETA:

$$SDFSBETA_{ij} = \left[\frac{Var\ (S_j(i)) - Var\ (S_j)}{Var\ (S_j)} \right]_{ij} , \quad (4)$$

where

$$Var\ (S) = \sigma^2 (A^T A)^{-1} , \text{ and} \quad (5)$$

$$Var\ (S(i)) = \sigma^2 (A^T A - a_i a_i^T)^{-1} \quad (6)$$

$$= \sigma^2 \left((A^T A)^{-1} + \frac{(A^T A)^{-1} a_i^T a_i (A^T A)^{-1}}{1 - a_i (A^T A)^{-1} a_i^T} \right) . \quad (7)$$

Note that σ in a properly defined CMB is 1.

2.1.2 Nondeletion diagnostics

The basis of the nondeletion diagnostic technique is an analysis of the degree of influence of the species on the predicted SCE and the variance of the SCE for the full model, i.e., without any deleted species.

Henry (1985) presented a complete error analysis of the CMB receptor model and showed the central role played by the weighted pseudo-inverse (PIN) of the source composition

matrix. Two diagnostic tools are developed based on the PIN.

The first diagnostic, SPINBETA, is the fraction of the predicted SCE contributed by the given species as shown by the PIN matrix. The second diagnostic is the fraction of the variance in the SCE contributed by a given species as indicated by the square of the PIN. Both diagnostics are normalized to be less than or equal to one in absolute value. As before, the closer the diagnostic is to one, the more influential the species.

2.1.2.1 SPINBETA

The weighted pseudo-inverse matrix(PIN) of source composition matrix is defined by

$$P_A = (A^T W A)^{-1} A^T W \qquad (8)$$

where A is the source composition matrix and W is matrix of weights for CMB. The matrix product of the PIN matrix and ambient concentrations column vector, C, gives the estimated SCEs,

$$S_j = \sum_{i}^{n} p_{ij} C_i, \qquad j = 1,2,\ldots,p \qquad (9)$$

where p_{ij} is the ij species of the PIN and C_i is the concentration of the i^{th} species. From this, it is clear that the fraction of the predicted SCE for source j contributed by

species i is,

$$SPINBETA_{ij} = \left[\frac{P_{ij} \times C_i}{S_j} \right]_{ij} \quad . \qquad (10)$$

This defines the first nondeletion diagnostic.

2.1.2.2 SPINSBETA

It is also of interest to find the influential species based on the variance of SCE. Henry (1985) derived the equation for the variance of the SCEs using the PIN matrix. The variance of the SCEs is the product of terms involving the squared species of the PIN matrix and the effective variances. Therefore, the contribution to the variance of the SCE of each species for each source is given by the matrix formed from the product of the squared species of the PIN matrix and the effective variances. This matrix is normalized to the variance of SCE to give the second nondeletion diagnostics:

$$SPINSBETA_{ij} = \left[\frac{P_{ij}^2 \times \sigma_{eff,i}^2}{Var\ (S_j)} \right]_{ij} \quad . \qquad (11)$$

2.2 Modified PIN matrix (MPIN)

In the previous section, four diagnostic tools were developed including both deletion diagnostics and nondeletion diagnostics. However, careful examination of the defining equations shows that each of these four diagnostics is either

exactly or approximately proportional to the modified PIN matrix (MPIN) as defined by:

$$MPIN = (A^T W A)^{-1} A^T W^{1/2} \quad . \qquad (12)$$

Note that the MPIN only differs from the PIN by a factor of $W^{1/2}$. This difference, however, is critical.

2.2.1 Comparisons of MPIN with other diagnostics

The equations for diagnostics are more easily compared with the MPIN if the weighted matrix, W, is incorporated as a factor of $W^{1/2}$ in the source matrix and ambient data vector. For example, equation 11 then becomes,

$$SPINSBETA_{ij} = \left[\frac{\bar{P}_{ij}^2}{Var\ (S_j)} \right]_{ij} \quad . \qquad (13)$$

where $\bar{P}_{ij}$ is the MPIN. Therefore, the species of SPINSBETA are exactly the squared species of MPIN. Similarly, there are only slight differences, between the mathematical equations for the three other diagnostics and MPIN. In SPINBETA, the weighted C vector is the additional term to MPIN. In SDFBETA, standardized residual $[e_i/(1-h_i)]$ is the extra part to MPIN. Finally, the inverse of variance of the residual $[1/(1-h_i)]$ in SDFSBETA is the only extra term to MPIN.

Table A2 - Table A7 in appendix compares the four diagnostics and the MPIN diagnostic. Each diagnostic is

normalized to the largest value for each source. All diagnostics, therefore, are always less than or equal to one and closer it is to one, the greater the influence of that species on a given source.

As shown in Table A2 - Table A7, SDFBETA is unstable to errors even if little or no collinearity between source profiles is present. This instability is caused by the extra residual part in SDFBETA. Therefore, SDFBETA is not recommended as a diagnostic tool.

SPINBETA gives almost the same information as MPIN does because the only different term in SPINBETA, ambient data vector C, is weighted. As explained before, the species of SPINSBETA is exactly the square of the species of MPIN. However, as can be seen in Table A2 - Table A7, SPINSBETA and MPIN do not always give exactly the same number because they are normalized to the largest value for each source.

Experience has shown that the extra term to MPIN in SDFSBETA, variance of the residual, does not provide extra information. As a result, SPINBETA, SPINSBETA and SDFSBETA are redundant in the sense that they provide little additional information and require much extra computation time. Therefore, this study simply adopted MPIN as a new diagnostic tool for detecting influential species for CMB receptor model.

Since the MPIN represents the above three diagnostics inherently, influential species detected by MPIN are

important species in terms of deletion and nondeletion diagnostics. MPIN is especially well suited to the CMB receptor model because it does not require extra calculation time, but can be obtained automatically during the SCE calculation.

A series of Monte Carlo simulations were performed to verify the above results and to determine a suitable cut-off value for MPIN at which a species is considered to be influential. The simulations are described below, followed by final conclusions and specific recommendations on the interpretation of MPIN.

3. Generation of simulated data sets

The purpose of the simulated data sets is to produce an experience base of results for known levels of error in the model. Although the simulation runs are called Monte Carlo simulations, their results are not intended to estimate any parameter with any accuracy. Thus, the results are to be evaluated in a qualitative and comparative fashion.

3.1 Background

Simulated data were generated as the same way as the previous study using the matrix equation,

$$C = (A + \epsilon_A) S^O + \epsilon_C \qquad (14)$$

where C is the vector of ambient chemical species concentrations, A is the matrix of source compositions, and S^o is the vector of the true SCE. Lognormal random errors (ϵ_A) were introduced to the source matrix and normally distributed measurement errors (ϵ_C) were introduced to the ambient concentrations.

The source compositions were taken from the Portland Aerosol Characterization Study (PACS). Two groups of sources were used for this study, PACS 1 and PACS 3. As shown in Table 1 and 2, the sources in PACS 1 are Marine, Urban dust(Udust), Auto, Residual oil (Rdoil), Kraft, Aluminum production (Alpro), Steel, and Ferromanganese (FeMn). The PACS 3 set consists of Marine, Urban dust (Udust), Auto and Residual oil (Rdoil) sources. Each source vector has 21 species with concentrations representative of fine particle aerosol. PACS 1 and PACS 3 source composition matrices are presented in Table 1 and Table 2 respectively. Typical values assumed for true SCE are given in Table 3.

3.2 Approach

Three sets of source composition matrix were created from the original composition matrix with uncertainties of 10%, 30%, and 50%. Similarly, three corresponding ambient data sets were produced with uncertainties of 10%. This means that the standard deviation of the errors was taken to be 10% of the mean value of the chemical species concentrations, C_i.

Table 1. Fractional Fine Particle Compositions of Eight Source Types.(PACS 1)

SPECIES	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	0.000000	0.118000	0.500000	0.070000	0.017000	0.039000	0.000000	0.090000
EC	0.000000	0.018500	0.038000	0.031000	0.002200	0.023000	0.000000	0.015000
NO_3	0.000000	0.000000	0.009100	0.006500	0.000000	0.004100	0.000000	0.057000
SO_4	0.100000	0.004200	0.013000	0.481000	0.400000	0.044000	0.025000	0.042000
Na	0.400000	0.012500	0.000000	0.035000	0.127000	0.041000	0.012600	0.031000
Mg	0.048000	0.013000	0.000000	0.000000	0.006300	0.028000	0.065000	0.000000
Al	0.000000	0.088400	0.011000	0.005300	0.002500	0.270000	0.006500	0.006400
Si	0.000000	0.223000	0.008200	0.009600	0.001500	0.003400	0.050000	0.009900
Cl	0.400000	0.000000	0.030000	0.000000	0.018000	0.013300	0.018500	0.004200
K	0.014000	0.010300	0.000720	0.002800	0.015000	0.002200	0.009200	0.105000
Ca	0.014000	0.024400	0.012500	0.015800	0.000000	0.003300	0.062000	0.013000
Ti	0.000000	0.006400	0.000000	0.001100	0.000060	0.000400	0.002000	0.000460
V	0.000000	0.000230	0.000000	0.034400	0.000010	0.000640	0.000600	0.000240
Cr	0.000000	0.000450	0.000000	0.000470	0.002800	0.000000	0.021000	0.000420
Mn	0.000000	0.001230	0.000000	0.000460	0.000300	0.000110	0.087000	0.173000
Fe	0.000000	0.060000	0.021000	0.029700	0.012000	0.004500	0.320000	0.021000
Ni	0.000000	0.000093	0.000180	0.053600	0.001300	0.001900	0.007000	0.000000
Cu	0.000000	0.000300	0.000730	0.000750	0.000210	0.000440	0.002800	0.000360
Zn	0.000000	0.001100	0.003500	0.004000	0.000690	0.000150	0.012000	0.005800
Br	0.002000	0.000200	0.050000	0.000130	0.001300	0.000370	0.000000	0.001600
Pb	0.000000	0.003700	0.200000	0.001100	0.000130	0.000120	0.007600	0.000450

Table 2. Fractional Fine Particle Compositions of Four Source Types. (PACS 3)

SPECIES	MARINE	UDUST	AUTO	RDOIL
OC	0.000000	0.118000	0.500000	0.070000
EC	0.000000	0.018500	0.038000	0.031000
NO_3	0.000000	0.000000	0.009100	0.006500
SO_4	0.100000	0.004200	0.013000	0.481000
Na	0.400000	0.012500	0.000000	0.035000
Mg	0.048000	0.013000	0.000000	0.000000
Al	0.000000	0.088400	0.011000	0.005300
Si	0.000000	0.223000	0.008200	0.009600
Cl	0.400000	0.000000	0.030000	0.000000
K	0.014000	0.010300	0.000720	0.002800
Ca	0.014000	0.024400	0.012500	0.015800
Ti	0.000000	0.006400	0.000000	0.001100
V	0.000000	0.000230	0.000000	0.034400
Cr	0.000000	0.000450	0.000000	0.000470
Mn	0.000000	0.001230	0.000000	0.000460
Fe	0.000000	0.060000	0.021000	0.029700
Ni	0.000000	0.000093	0.000180	0.053600
Cu	0.000000	0.000300	0.000730	0.000750
Zn	0.000000	0.001100	0.003500	0.004000
Br	0.002000	0.000200	0.050000	0.000130
Pb	0.000000	0.003700	0.200000	0.001100

Table 3. Source Contributions Chosen as the True Value

PACS 1	MARINE = 2	(μg/m3)
	UDUST = 35	
	AUTO = 10	
	RDOIL = 5	
	KRAFT = 5	
	ALPRO = 5	
	STEEL = 10	
	FeMn = 5	
PACS 3	MARINE = 2	
	UDUST = 35	
	AUTO = 10	
	RDOIL = 5	

Unlike the normal distribution, the lognormal distribution, used to generate errors in the source matrix, is skew symmetric and the meaning of 10%, 30%, and 50% error is not obvious. If g_m is the geometric mean and σ_g is the geometric standard deviation, then an uncertainty (or error) of e% is defined by the equation,

$$\left(\frac{\sigma_g^2 g_m - g_m}{g_m} \right) \times 100 = e\% \qquad (15)$$

With this definition, an error of 50% implies that the 2 sigma point of the error of the error distribution is 50% above the mean.

The geometric standard deviation, $\sigma_g = \sqrt{1 + e/100}$, is easily obtained from the above equation when e% error is allowed. This geometric standard deviation must be converted to the arithmetic standard deviation when used in calculating effective variance weights. Zeroes in the source compositions matrix were replaced by a small number 10^{-6}, for purposes of calculating a percentage error. The characteristics of data sets are given in Table 4.

As stated at the beginning of this section, these simulations are not intended to estimate any parameter with great accuracy. They are only meant to provide a base of results with which to compare the performance of the various diagnostics in a qualitative or semi-quantitative manner. Three repetitions of each simulation were found to be

Table 4. Data Set Characteristics

Simulated data Sets	True Source Matrix Chosen	Number of Source Types	Number of Species	Uncertainty Level(Aij)	Uncertainty Level(Ci)
SET 1	PACS 1	8	21	10%	10%
SET 2	PACS 1	8	21	30%	10%
SET 3	PACS 1	8	21	50%	10%
SET 4	PACS 3	4	21	10%	10%
SET 5	PACS 3	4	21	30%	10%
SET 6	PACS 3	4	21	50%	10%

sufficient for this purpose. As a practical matter, carrying out 400 repetitions, say, would have made it impossible to test as many different cases as we did.

3.3 Procedure

The simulated data sets are created as follows.

In the following, the superscript ^{o} denotes the "true" or unperturbed value.

1). Simulate the errors in source matrix using random numbers drawn from a lognormal distribution of geometric mean a_{ij} and geometric standard deviation $\sigma_g = \sqrt{1 + e/100}$.

$$a_{ij}^{o} = a_{ij} + \epsilon_A \qquad (16)$$

where e refers to the percent errors in source matrix as defined in equation 15.

2). Generate true concentrations using a model which represents the situation under study using,

$$C_i^{o} = \Sigma\, a_{ij}^{o} S_j^{o} , \qquad i = 1,.....,N \qquad (17)$$

3). Simulate the measurement process to obtain measured value of C_i using random numbers drawn from a normal distribution of mean 0 and standard deviation of $0.1C_i^{o}$:

$$C_i = C_i^{o} + \epsilon_C \qquad (18)$$

4). Obtain weights to be used in the effective variance weighted least squares method.

$$W_i^2 = \sigma_{ci}^2 + \Sigma\ \sigma_{aij}^2\ S_j^2 \qquad (19)$$

where $\sigma_{ci} = 0.1C_i^{o}$ and σ_{aij} is an arithmetic standard deviation. Therefore, geometric standard deviation (σ_g) has to be converted to arithmetic standard deviation (σ_{aij}) with the following relationships.

$$\sigma_{aij} = \text{mean} \times [\exp(\ln^2\sqrt{1+e/100}) - 1]^{1/2}, \text{ and} \qquad (20)$$

$$\text{mean} = a_{ij}\ \exp[0.5 \times \ln^2\sqrt{1+e/100}\ ] \qquad (21)$$

4. Effective variance weighted least squares method

All tests used the effective variance weighted least squares method. Since the effective variance method depends on the SCE which are unknown, an iterative procedure is required. At each iteration, the previously estimated S_j are used to compute new effective variance weights which are used, in turn, to compute new S_j. The iteration process terminates when the S_j do not change more than 1% from step to step. Therefore, the iteration process terminates with confidence that the additional steps will not improve S_j by more than 1%.

5. Results

For each data set, results are summarized in the Appendices. The following observations can be made from the results.

Tables 5 and 6 are examples of the analysis applied to the results in the Appendices. Table 5 gives the influential species as determined by the five diagnostics under consideration for the data set 3 simulations, i.e., eight sources, large collinearity, 50% error in the source matrix and 10% error in the observations. The Table also gives the coefficient of variation of the diagnostics, this is a good, rough measure of the stability of the diagnostic to errors. SDFBETA is seen by this measure to be rather unstable, while the other measures are quite stabile. Comparison of the influential elements according to the various diagnostics shows a comfortingly high degree of agreement between them. Only SDFBETA has consistently different results, and this is undoubtedly caused by its instability.

Table 6 is the same as Table 5 but for simulation set 6, i.e., four sources, little collinearity, 50% error in the source matrix and 10% error in the measurements. The results as shown in this Table are the same as in Table 5. As a whole, the results in the Appendices also give the same results as enumerated below.

Table 5. Influential elements and their coefficient of variation by different diagnostics for data set 3.

	SDFBETA	SDFSBETA	SPINBETA	SPINSBETA	NMPIN
MARINE	Cl (.000)*	Cl (.000)	Cl (.000)	Cl (.000)	Cl (.000)
UDUST	OC (.360)	Si (.007)	Ti (.002)	Si (.004)	Si (.002)
	NO_3(.592)	Ti (.086)	Si (.050)	Ti (.060)	Ti (.030)
AUTO	Br (.087)	Br (.000)	Pb (.027)	Br (.000)	Br (.000)
	OC (.395)	Pb (.065)	Br (.123)	Pb (.038)	Pb (.019)
RDOIL	V (.309)	V (.000)	Ni (.000)	V (.000)	V (.000)
	Ni (.988)	Ni (.167)	V (.047)	Ni (.088)	Ni (.045)
KRAFT	SO_4(.000)	SO_4(.000)	SO_4(.000)	SO_4(.000)	SO_4(.000)
ALPRO	Al (.000)	Al (.000)	Al (.000)	Al (.000)	Al (.000)
STEEL	Cr (.751)	Cr (.000)	Cr (.182)	Cr (.000)	Cr (.000)
FeMn	NO_3(.000)	NO_3(.000)	NO_3(.000)	NO_3(.000)	NO_3(.000)

* coefficient of variation = standard deviation/mean of three simulation runs

Table 6. Influential elements and their coefficient of variation by different diagnostics for data set 6.

	SDFBETA	SDFSBETA	SPINBETA	SPINSBETA	NMPIN
MARINE	Cl (.000)*	Cl (.000)	Na (.000)	Cl (.000)	Cl (.000)
	Na (.404)	Na (.102)	Cl (.027)	Na (.057)	Na (.029)
UDUST	Mn (.454)	Si (.003)	Cr (.215)	Si (.002)	Si (.001)
	Cr (.176)	Ti (.056)	K (.032)	Ti (.050)	Ti (.025)
	Mg (.584)	Al (.036)	Ti (.104)	Al (.032)	Al (.017)
AUTO	Br (.108)	Br (.095)	Pb (.063)	Br (.070)	Br (.035)
	NO_3(.648)	Pb (.187)	NO_3(.236)	Pb (.139)	Pb (.068)
	Pb (.709)	NO_3(.151)	Br (.224)	NO_3(.131)	NO_3(.066)
RDOIL	Ni (.000)	Ni (.000)	V (.009)	Ni (.000)	Ni (.000)
	V (.643)	V (.131)	SO_4(.028)	V (.086)	V (.042)

* coefficient of variation = standard deviation/mean of three simulation runs

1) As was expected, SDFBETA is unstable to errors (Table A2-Table A7). Therefore, SDFBETA is not recommended as a diagnostic tool.
2) SDFSBETA, SPINBETA, and SPINSBETA give almost the same information as MPIN does (Table A2 - Table A7). Therefore, MPIN can be used as a new diagnostic tool representing above three diagnostics implicitly.
3) Influential species detected by MPIN are, therefore, important species in determining SCE and their variances in CMB receptor model.
4) In general, influential species are not specific to certain type of sources but are dependent on the mix of sources chosen in the CMB.
5) Number of influential species for certain type of source is often only one or two, but sometimes can be more than this.
6) When there are several influential species, deletion of some (but not all) of these species may not drastically affect the SCE or their variance. However, deletion of all of the influential species detected has drastic effects on the SCE and its variance (Table A8).
7) As was expected, deletion of some or all the noninfluential species identified by MPIN has little affect on the SCE and their variances (Table A8).

6. Conclusions and recommendations

A new diagnostic tool, MPIN, was developed and tested for its ability to detect influential species for CMB applications. The MPIN diagnostic gives the relative importance of the species for each source both in determining the SCE and their variances. Unfortunately, there can be no universal rule for cutoff value to detect which species are influential and which species are not. The definition of "influential" is somewhat arbitrary and subjective and dependent on the specific application. The following guidelines for use of the MPIN diagnostic are based on experience gained in this project and are recommended as guidelines for interpreting the normalized MPIN.

1) Species having normalized MPIN number of greater than 0.5 are considered to be influential,
2) Species having normalized MPIN number of between 0.3 and 0.5 are considered to be intermediate, and
3) Species having normalized MPIN number of less than 0.3 are considered to be noninfluential.

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Appendix

Results of each data set are summarized in Tables as shown below:

PACS 1	Set 3*	Table A1	: Listing of whole output
PACS 1	Set 1	Table A2	:
	Set 2	Table A3	: Comparisons of MPIN with
	Set 3	Table A4	: other diagnostics
PACS 3	Set 4	Table A5	:
	Set 5	Table A6	: Comparisons of MPIN with
	Set 6	Table A7	: other diagnostics
PACS 3	Set 6	Table A8	: Effects of deletion of influential and noninfluential elements

* Characteristics of data set is given in Table 4.

In Table A1 - Table A7, NMPIN is the normalized MPIN. MEAN- and STD- represent the mean and standard deviation of three simulation runs. For example, MEANNMPIN is the mean value of NMPIN for three runs.

Table A1. Complete listing of three simulation runs for data set 3

EIGENVALUES

2.564	2.084	1.213	.680	.562	.194	.129	-.036

INVERSE SINGULAR VALUE

.625	.693	.908	1.213	1.334	2.273	2.779	5.238

EIGENVECTORS

MARINE	.701	-.669	-.168	-.050	-.054	-.164	-.019	.020
UDUST	.041	.005	.072	.065	.107	.077	.454	.875
AUTO	.106	-.010	.246	.951	-.127	.003	-.081	-.039
RDOIL	.618	.741	-.207	-.019	-.087	-.135	-.005	.010
KRAFT	.205	-.004	-.007	-.044	-.023	.953	-.217	.026
ALPRO	.091	-.008	.045	.038	.055	.190	.850	-.476
STEEL	.182	.043	.342	-.001	.908	-.042	-.129	-.077
FeMn	.176	.033	.863	-.293	-.367	-.057	-.015	.000

VARIANCE AND COVARIANCE MATRIX

MARINE	.591	.330	-.070	.090	-.695	-.533	-.087	.025
UDUST	.330	22.645	-1.128	.155	.229	-8.342	-2.114	-.124
AUTO	-.070	-1.128	1.505	-.036	.073	.027	.032	-.136
RDOIL	.090	.155	-.036	.560	-.597	-.302	-.127	.013
KRAFT	-.695	.229	.073	-.597	5.091	-.821	-.068	-.214
ALPRO	-.533	-8.342	.027	-.302	-.821	11.993	.219	-.163
STEEL	-.087	-2.114	.032	-.127	-.068	.219	1.875	-.308
FeMn	.025	-.124	-.136	.013	-.214	-.163	-.308	1.011

STANDARD ERROR OF REGRESSION COEFFICIENT

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
.768	4.759	1.227	.748	2.256	3.463	1.369	1.005

SOURCE STRENGTH

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
3.426	33.570	7.899	4.188	6.419	8.211	10.277	5.530

Table A1. Continued

SDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.015	.898	1.000	.016	.014	.176	.230	.000
EC	.025	.438	.260	.044	.026	.161	.169	.011
NO_3	.017	.730	.277	.070	.137	.349	.432	1.000
SO_4	.356	.176	.063	.050	1.000	.027	.130	.077
Na	.431	.169	.265	.120	.343	.079	.195	.007
Mg	.048	.252	.205	.104	.055	.567	.707	.139
Al	.109	.174	.158	.074	.062	1.000	.130	.041
Si	.006	.295	.047	.003	.001	.069	.040	.003
Cl	1.000	.154	.195	.099	.317	.130	.008	.006
K	.016	1.000	.421	.046	.113	.318	.356	.645
Ca	.024	.616	.052	.013	.018	.167	.163	.021
Ti	.007	.375	.065	.006	.001	.084	.047	.003
V	.125	.118	.148	1.000	.322	.087	.193	.014
Cr	.080	.508	.014	.105	.096	.016	1.000	.126
Mn	.010	.386	.157	.032	.045	.025	.403	.397
Fe	.006	.142	.021	.009	.003	.057	.183	.026
Ni	.030	.173	.039	.414	.119	.034	.096	.022
Cu	.074	.352	.264	.030	.006	.188	.790	.093
Zn	.042	.165	.342	.019	.008	.138	.921	.052
Br	.017	.189	.855	.014	.014	.004	.003	.024
Pb	.004	.032	.199	.002	.002	.003	.004	.007

SDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.152	.185	.000	.000	.005	.053	.000
EC	.001	.086	.030	.005	.001	.010	.068	.000
NO_3	.000	.064	.009	.003	.005	.013	.119	1.000
SO_4	.178	.014	.002	.006	1.000	.000	.040	.022
Na	.075	.004	.009	.010	.034	.001	.025	.000
Mg	.001	.008	.005	.008	.001	.036	.338	.020
Al	.043	.034	.028	.034	.010	1.000	.101	.016
Si	.001	1.000	.025	.001	.000	.049	.097	.001
Cl	1.000	.007	.012	.017	.072	.005	.000	.000
K	.000	.123	.021	.001	.004	.011	.083	.425
Ca	.001	.180	.001	.000	.000	.012	.067	.002
Ti	.001	.904	.026	.001	.000	.040	.077	.001
V	.009	.003	.004	1.000	.043	.001	.036	.000
Cr	.004	.048	.000	.012	.004	.000	1.000	.025
Mn	.000	.041	.007	.002	.001	.000	.241	.365
Fe	.000	.042	.001	.001	.000	.006	.368	.011
Ni	.002	.016	.001	.522	.018	.001	.027	.002
Cu	.003	.019	.011	.001	.000	.005	.508	.011
Zn	.000	.002	.007	.000	.000	.001	.286	.001
Br	.001	.050	1.000	.002	.001	.000	.000	.007
Pb	.001	.022	.808	.001	.000	.000	.002	.010

Table A1. Continued

SPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.019	.473	.611	.025	.016	.124	.224	.001
EC	.064	.482	.332	.137	.062	.237	.344	.031
NO_3	.016	.286	.126	.078	.115	.182	.314	1.000
SO_4	.394	.082	.034	.067	1.000	.017	.113	.093
Na	.564	.093	.171	.190	.406	.059	.200	.010
Mg	.056	.123	.117	.145	.058	.370	.642	.173
Al	.194	.131	.138	.158	.099	1.000	.180	.079
Si	.047	.993	.184	.032	.010	.311	.249	.022
Cl	1.000	.065	.096	.120	.287	.073	.006	.006
K	.015	.397	.194	.052	.096	.168	.263	.654
Ca	.061	.674	.066	.041	.042	.243	.330	.059
Ti	.046	1.000	.201	.043	.004	.299	.234	.023
V	.091	.037	.053	.883	.213	.036	.111	.011
Cr	.072	.195	.006	.115	.079	.008	.714	.124
Mn	.014	.232	.109	.055	.058	.020	.449	.608
Fe	.026	.270	.047	.051	.013	.145	.645	.124
Ni	.060	.147	.038	1.000	.215	.039	.151	.048
Cu	.119	.240	.209	.058	.008	.171	1.000	.162
Zn	.043	.072	.172	.024	.008	.080	.741	.058
Br	.041	.190	1.000	.041	.031	.005	.005	.061
Pb	.041	.139	.988	.030	.014	.017	.035	.082

SPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.181	.253	.000	.000	.018	.058	.000
EC	.003	.108	.043	.009	.003	.038	.079	.001
NO_3	.000	.049	.008	.004	.015	.029	.084	1.000
SO_4	.123	.004	.001	.002	1.000	.000	.010	.008
Na	.181	.003	.009	.014	.118	.002	.021	.000
Mg	.003	.009	.007	.013	.004	.123	.364	.031
Al	.039	.012	.011	.017	.013	1.000	.032	.007
Si	.003	1.000	.029	.001	.000	.142	.090	.001
Cl	1.000	.003	.005	.010	.104	.005	.000	.000
K	.000	.125	.025	.002	.014	.033	.078	.571
Ca	.003	.233	.002	.001	.002	.044	.080	.003
Ti	.003	.933	.031	.002	.000	.121	.073	.001
V	.016	.002	.003	1.000	.110	.002	.022	.000
Cr	.011	.052	.000	.019	.016	.000	1.000	.035
Mn	.000	.041	.008	.002	.005	.000	.222	.478
Fe	.001	.052	.001	.002	.000	.022	.424	.018
Ni	.004	.015	.001	.689	.060	.001	.022	.003
Cu	.009	.023	.015	.001	.000	.017	.580	.018
Zn	.001	.002	.011	.000	.000	.004	.351	.003
Br	.003	.043	1.000	.002	.002	.000	.000	.007
Pb	.003	.021	.880	.001	.000	.000	.002	.012

Table A1. Continued

NMPIN	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.021	.425	.503	.022	.020	.134	.242	.001
EC	.054	.328	.207	.094	.059	.194	.281	.028
NO_3	.015	.220	.089	.061	.123	.169	.290	1.000
SO_4	.351	.059	.023	.049	1.000	.015	.098	.087
Na	.425	.057	.095	.117	.344	.043	.147	.008
Mg	.054	.097	.084	.115	.063	.350	.604	.177
Al	.198	.108	.104	.132	.114	1.000	.179	.085
Si	.059	1.000	.170	.032	.014	.377	.300	.029
Cl	1.000	.053	.071	.098	.322	.072	.006	.007
K	.017	.354	.158	.047	.118	.181	.280	.755
Ca	.054	.483	.043	.030	.042	.210	.283	.055
Ti	.054	.966	.177	.042	.006	.348	.271	.029
V	.127	.041	.054	1.000	.332	.049	.149	.016
Cr	.104	.228	.007	.136	.128	.012	1.000	.187
Mn	.015	.203	.087	.049	.071	.022	.471	.692
Fe	.027	.228	.036	.043	.016	.148	.651	.135
Ni	.060	.121	.029	.830	.246	.039	.149	.052
Cu	.094	.153	.122	.037	.007	.131	.761	.133
Zn	.036	.048	.105	.016	.007	.064	.593	.050
Br	.055	.208	1.000	.046	.047	.007	.007	.087
Pb	.053	.144	.938	.032	.020	.021	.044	.110

Table A1. Continued

EIGENVALUES

3.248	1.543	1.141	.587	.531	.188	.136	.029

INVERSE SINGULAR VALUE

.555	.805	.936	1.305	1.373	2.309	2.714	5.869

EIGENVECTORS

MARINE	.957	-.241	-.003	-.055	-.016	-.153	-.009	.018
UDUST	.026	.058	.033	.121	.021	.105	.393	.902
AUTO	.076	.143	.136	.334	.912	.029	-.094	-.044
RDOIL	.132	.714	-.629	-.129	.029	-.245	.021	.009
KRAFT	.179	.162	-.133	-.069	-.052	.915	-.280	.015
ALPRO	.078	.070	.009	.063	.019	.250	.863	-.421
STEEL	.107	.285	.166	.837	-.399	-.040	-.113	-.077
FeMn	.108	.545	.735	-.381	-.065	-.049	-.017	.001

VARIANCE AND COVARIANCE MATRIX

MARINE	.461	.420	-.104	.145	-.685	-.511	-.085	.025
UDUST	.420	29.270	-1.521	.188	.152	-10.432	-2.561	-.083
AUTO	-.104	-1.521	1.927	-.096	.187	.162	.029	-.184
RDOIL	.145	.188	-.096	1.039	-1.068	-.309	-.150	-.007
KRAFT	-.685	.152	.187	-1.068	5.108	-.770	-.044	-.175
ALPRO	-.511	-10.432	.162	-.309	-.770	11.939	.434	-.201
STEEL	-.085	-2.561	.029	-.150	-.044	.434	1.879	-.261
FeMn	.025	-.083	-.184	-.007	-.175	-.201	-.261	.939

STANDARD ERROR OF REGRESSION COEFFICIENT

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
.679	5.410	1.388	1.019	2.260	3.455	1.371	.969

SOURCE STRENGTH

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
2.540	39.583	9.261	6.060	3.085	2.689	10.185	5.209

Table A1. Continued

SDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.031	1.000	.964	.051	.036	.581	.748	.063
EC	.014	.236	.119	.154	.032	.126	.240	.002
NO_3	.009	.234	.079	.119	.075	.261	.302	1.000
SO_4	.403	.154	.071	.333	1.000	.027	.201	.166
Na	.225	.076	.088	.304	.248	.064	.191	.016
Mg	.000	.001	.001	.003	.001	.008	.013	.003
Al	.082	.063	.049	.114	.047	1.000	.134	.072
Si	.010	.226	.033	.010	.001	.146	.096	.004
Cl	1.000	.115	.115	.390	.371	.160	.058	.023
K	.004	.212	.077	.072	.040	.178	.177	.389
Ca	.026	.365	.033	.059	.021	.261	.197	.031
Ti	.043	.952	.150	.071	.002	.596	.383	.019
V	.033	.011	.022	.547	.084	.020	.053	.003
Cr	.005	.017	.000	.017	.006	.002	.093	.012
Mn	.003	.057	.025	.028	.010	.005	.181	.197
Fe	.013	.349	.053	.065	.009	.331	1.000	.154
Ni	.046	.066	.032	1.000	.145	.034	.084	.037
Cu	.008	.021	.015	.001	.000	.028	.132	.018
Zn	.003	.007	.017	.014	.002	.017	.140	.010
Br	.063	.266	1.000	.153	.053	.053	.009	.146
Pb	.027	.088	.444	.055	.016	.001	.024	.079

SDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.179	.224	.000	.000	.007	.054	.000
EC	.000	.103	.035	.011	.002	.004	.057	.000
NO_3	.000	.109	.017	.007	.011	.016	.098	1.000
SO_4	.166	.025	.007	.030	1.000	.000	.023	.015
Na	.063	.008	.014	.030	.076	.001	.026	.000
Mg	.000	.006	.006	.006	.001	.029	.299	.013
Al	.054	.033	.026	.027	.017	1.000	.081	.022
Si	.002	1.000	.029	.001	.000	.050	.097	.000
Cl	1.000	.014	.019	.040	.135	.003	.002	.000
K	.000	.183	.032	.005	.006	.016	.069	.309
Ca	.001	.201	.002	.001	.001	.012	.031	.001
Ti	.002	.843	.028	.001	.000	.040	.073	.000
V	.014	.002	.009	1.000	.087	.001	.020	.000
Cr	.005	.065	.000	.016	.007	.000	1.000	.016
Mn	.000	.035	.009	.002	.001	.000	.196	.215
Fe	.000	.063	.002	.001	.000	.007	.278	.006
Ni	.005	.011	.004	.661	.052	.000	.010	.002
Cu	.002	.018	.013	.000	.000	.004	.397	.007
Zn	.000	.002	.011	.002	.000	.001	.318	.001
Br	.003	.052	1.000	.004	.002	.000	.000	.008
Pb	.002	.027	.919	.003	.001	.000	.001	.011

Table A1. Continued

SPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.021	.448	.513	.014	.024	.162	.246	.023
EC	.046	.487	.291	.194	.098	.162	.364	.003
NO_3	.017	.293	.118	.091	.139	.203	.278	1.000
SO_4	.417	.104	.057	.138	1.000	.011	.100	.090
Na	.481	.107	.146	.260	.513	.056	.197	.017
Mg	.033	.107	.111	.131	.068	.420	.753	.179
Al	.202	.101	.093	.112	.112	1.000	.158	.093
Si	.064	.914	.159	.026	.006	.368	.285	.014
Cl	1.000	.075	.090	.156	.359	.065	.028	.012
K	.016	.543	.234	.113	.151	.285	.334	.796
Ca	.073	.660	.071	.065	.056	.294	.262	.045
Ti	.070	1.000	.188	.046	.003	.390	.296	.016
V	.145	.030	.074	.953	.352	.036	.111	.007
Cr	.111	.256	.007	.156	.127	.015	1.000	.144
Mn	.016	.219	.115	.066	.055	.011	.515	.607
Fe	.017	.293	.053	.033	.011	.173	.617	.103
Ni	.116	.108	.062	1.000	.350	.035	.101	.049
Cu	.111	.197	.171	.004	.006	.168	.924	.137
Zn	.046	.060	.168	.074	.029	.092	.878	.067
Br	.081	.223	1.000	.079	.066	.028	.005	.098
Pb	.074	.159	.951	.060	.042	.002	.031	.114

SPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.205	.287	.000	.001	.028	.061	.001
EC	.001	.127	.048	.019	.007	.015	.070	.000
NO_3	.000	.069	.012	.006	.022	.035	.061	1.000
SO_4	.141	.008	.002	.012	1.000	.000	.007	.007
Na	.145	.006	.012	.034	.203	.002	.021	.000
Mg	.001	.007	.008	.010	.004	.113	.339	.024
Al	.044	.010	.009	.011	.017	1.000	.023	.010
Si	.006	1.000	.032	.001	.000	.171	.096	.000
Cl	1.000	.005	.007	.020	.159	.004	.001	.000
K	.000	.182	.036	.007	.020	.053	.068	.486
Ca	.004	.257	.003	.002	.003	.054	.040	.002
Ti	.005	.888	.033	.002	.000	.143	.076	.000
V	.029	.001	.007	1.000	.210	.002	.014	.000
Cr	.014	.066	.000	.023	.023	.000	1.000	.026
Mn	.000	.037	.011	.003	.003	.000	.203	.357
Fe	.000	.076	.003	.001	.000	.028	.333	.012
Ni	.013	.010	.003	.786	.148	.001	.008	.003
Cu	.008	.022	.018	.000	.000	.017	.480	.013
Zn	.001	.002	.016	.003	.001	.005	.391	.003
Br	.007	.047	1.000	.005	.006	.001	.000	.011
Pb	.006	.025	.949	.003	.002	.000	.001	.016

Table A1. Continued

NMPIN	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.023	.452	.536	.013	.028	.168	.247	.025
EC	.036	.357	.220	.137	.086	.122	.264	.002
NO_3	.017	.263	.109	.079	.149	.187	.247	1.000
SO_4	.375	.087	.050	.111	1.000	.010	.083	.084
Na	.380	.078	.111	.184	.451	.042	.144	.014
Mg	.028	.084	.089	.098	.063	.336	.582	.156
Al	.211	.098	.093	.105	.130	1.000	.153	.101
Si	.075	1.000	.180	.027	.008	.414	.310	.018
Cl	1.000	.070	.086	.140	.399	.063	.026	.012
K	.014	.426	.189	.085	.141	.229	.260	.697
Ca	.060	.507	.056	.048	.052	.232	.199	.039
Ti	.070	.942	.183	.042	.004	.378	.276	.017
V	.170	.033	.084	1.000	.458	.040	.120	.009
Cr	.120	.258	.007	.151	.153	.015	1.000	.162
Mn	.015	.193	.105	.056	.058	.010	.451	.598
Fe	.017	.276	.051	.030	.013	.168	.577	.109
Ni	.115	.099	.059	.886	.385	.033	.092	.050
Cu	.090	.149	.133	.003	.005	.130	.693	.115
Zn	.035	.043	.125	.051	.025	.068	.625	.054
Br	.084	.216	1.000	.073	.077	.028	.005	.106
Pb	.079	.157	.974	.058	.050	.002	.031	.127

Table A1. Continued

EIGENVALUES

3.586	2.189	1.254	.562	.508	.224	.181	.036

INVERSE SINGULAR VALUE

.528	.676	.893	1.334	1.403	2.115	2.353	5.248

EIGENVECTORS

MARINE	.953	-.234	-.102	-.059	.015	-.144	.039	.018
UDUST	.025	.031	.070	.129	-.065	.208	.323	.908
AUTO	.076	.049	.178	.816	.527	-.022	-.117	-.049
RDOIL	.175	.937	-.240	-.063	.073	-.146	.052	.011
KRAFT	.168	.119	.002	-.083	.007	.811	-.540	.010
ALPRO	.076	.048	.049	.098	-.033	.495	.755	-.405
STEEL	.103	.146	.303	.420	-.819	-.076	-.127	-.087
FeMn	.099	.160	.895	-.343	.200	-.071	.019	-.005

VARIANCE AND COVARIANCE MATRIX

MARINE	.403	.373	-.105	.085	-.592	-.362	-.103	.026
UDUST	.373	23.538	-1.321	.203	.023	-8.302	-2.261	-.205
AUTO	-.105	-1.321	1.904	-.060	.151	.126	.015	-.157
RDOIL	.085	.203	-.060	.587	-.613	-.228	-.167	.020
KRAFT	-.592	.023	.151	-.613	4.591	-.581	.016	-.248
ALPRO	-.362	-8.302	.126	-.228	-.581	8.798	.421	-.054
STEEL	-.103	-2.261	.015	-.167	.016	.421	2.044	-.327
FeMn	.026	-.205	-.157	.020	-.248	-.054	-.327	.967

STANDARD ERROR OF REGRESSION COEFFICIENT

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
.635	4.852	1.380	.766	2.143	2.966	1.430	.984

SOURCE STRENGTH

MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
2.341	33.610	9.408	4.393	6.100	.976	10.652	5.397

Table A1. Continued

SDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.008	.466	.435	.041	.008	.222	.108	.006
EC	.004	.180	.091	.110	.008	.057	.056	.003
NO_3	.010	1.000	.320	.552	.148	.816	.463	1.000
SO_4	.361	.323	.133	.458	1.000	.035	.086	.099
Na	.245	.184	.206	.668	.303	.113	.139	.002
Mg	.002	.027	.018	.064	.003	.101	.080	.013
Al	.039	.082	.058	.169	.028	1.000	.048	.014
Si	.005	.234	.027	.017	.000	.117	.027	.003
Cl	1.000	.229	.215	.730	.370	.202	.012	.008
K	.009	.747	.236	.154	.056	.463	.231	.391
Ca	.009	.369	.023	.032	.008	.204	.089	.014
Ti	.007	.341	.043	.032	.001	.165	.037	.004
V	.020	.032	.027	1.000	.052	.030	.039	.004
Cr	.078	.602	.002	.713	.092	.077	1.000	.124
Mn	.014	.503	.144	.240	.044	.062	.428	.359
Fe	.002	.059	.007	.028	.002	.045	.070	.010
Ni	.001	.003	.001	.045	.002	.001	.002	.000
Cu	.038	.235	.134	.129	.009	.204	.453	.052
Zn	.001	.005	.006	.000	.000	.004	.019	.001
Br	.035	.317	1.000	.158	.025	.044	.002	.035
Pb	.012	.089	.366	.049	.006	.001	.007	.016

SDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.133	.240	.000	.000	.005	.064	.000
EC	.000	.104	.055	.009	.001	.002	.089	.000
NO_3	.000	.079	.017	.006	.008	.009	.151	1.000
SO_4	.142	.023	.008	.011	1.000	.000	.015	.028
Na	.049	.006	.015	.017	.068	.000	.029	.000
Mg	.000	.006	.006	.008	.000	.014	.493	.020
Al	.045	.041	.042	.041	.021	1.000	.126	.015
Si	.002	.988	.028	.001	.000	.040	.120	.002
Cl	1.000	.011	.020	.025	.126	.001	.000	.000
K	.000	.156	.032	.002	.004	.010	.134	.540
Ca	.001	.180	.001	.000	.000	.009	.093	.003
Ti	.002	1.000	.033	.002	.000	.038	.105	.002
V	.008	.004	.007	1.000	.053	.001	.060	.001
Cr	.003	.040	.000	.013	.004	.000	1.000	.022
Mn	.000	.053	.009	.003	.002	.000	.343	.343
Fe	.000	.039	.001	.002	.000	.004	.491	.015
Ni	.002	.016	.003	.732	.031	.001	.032	.002
Cu	.003	.020	.014	.001	.000	.002	.675	.013
Zn	.001	.004	.012	.000	.000	.000	.497	.001
Br	.003	.049	1.000	.003	.001	.000	.000	.007
Pb	.002	.025	.876	.002	.001	.000	.001	.011

Table A1. Continued

SPINBETA	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.036	.574	.786	.027	.028	.223	.284	.019
EC	.039	.458	.340	.146	.059	.119	.301	.023
NO_3	.012	.371	.174	.107	.162	.247	.366	1.000
SO_4	.419	.109	.066	.081	1.000	.010	.062	.091
Na	.537	.118	.193	.223	.571	.059	.190	.003
Mg	.032	.106	.100	.129	.036	.319	.660	.140
Al	.162	.101	.104	.108	.100	1.000	.125	.046
Si	.068	1.000	.171	.037	.001	.408	.248	.030
Cl	1.000	.067	.092	.111	.319	.048	.007	.006
K	.020	.461	.213	.049	.102	.234	.303	.650
Ca	.059	.683	.062	.031	.044	.308	.349	.069
Ti	.067	.996	.185	.049	.005	.394	.229	.030
V	.127	.058	.074	.964	.285	.046	.155	.018
Cr	.126	.283	.001	.175	.127	.030	1.000	.158
Mn	.022	.237	.100	.059	.061	.024	.430	.457
Fe	.038	.281	.052	.070	.023	.174	.713	.131
Ni	.080	.138	.056	1.000	.264	.050	.137	.035
Cu	.098	.177	.148	.051	.019	.125	.725	.106
Zn	.069	.097	.176	.001	.001	.059	.793	.030
Br	.065	.173	.801	.045	.041	.020	.002	.051
Pb	.080	.167	1.000	.048	.033	.002	.026	.083

SPINSBETA	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.156	.311	.000	.001	.026	.066	.000
EC	.001	.128	.075	.015	.003	.009	.096	.001
NO_3	.000	.061	.014	.006	.019	.029	.102	1.000
SO_4	.141	.007	.003	.005	1.000	.000	.004	.011
Na	.131	.005	.014	.020	.185	.001	.022	.000
Mg	.001	.008	.007	.013	.001	.076	.513	.030
Al	.031	.009	.010	.013	.015	1.000	.025	.004
Si	.006	.994	.031	.002	.000	.180	.105	.002
Cl	1.000	.003	.007	.011	.127	.002	.000	.000
K	.000	.146	.033	.002	.012	.041	.109	.658
Ca	.002	.230	.002	.001	.002	.051	.104	.005
Ti	.006	1.000	.037	.003	.000	.171	.091	.002
V	.019	.003	.005	1.000	.120	.002	.038	.001
Cr	.012	.046	.000	.021	.015	.001	1.000	.033
Mn	.001	.053	.010	.004	.006	.001	.299	.445
Fe	.001	.047	.002	.003	.000	.020	.525	.023
Ni	.006	.013	.002	.818	.078	.002	.022	.002
Cu	.010	.025	.018	.002	.000	.014	.718	.020
Zn	.003	.005	.017	.000	.000	.002	.546	.001
Br	.008	.044	1.000	.004	.004	.001	.000	.009
Pb	.007	.024	.921	.002	.002	.000	.001	.014

Table A1. Continued

NMPIN	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.028	.395	.557	.020	.025	.161	.256	.019
EC	.035	.358	.274	.124	.059	.097	.309	.028
NO_3	.009	.246	.119	.077	.137	.171	.319	1.000
SO_4	.376	.086	.053	.069	1.000	.008	.064	.107
Na	.362	.070	.118	.143	.430	.037	.147	.003
Mg	.030	.088	.086	.116	.037	.276	.716	.174
Al	.177	.096	.102	.112	.122	1.000	.157	.067
Si	.077	.997	.176	.040	.001	.424	.325	.045
Cl	1.000	.059	.083	.106	.356	.044	.008	.008
K	.019	.381	.182	.044	.108	.202	.330	.811
Ca	.047	.480	.045	.024	.039	.226	.322	.073
Ti	.077	1.000	.192	.053	.007	.413	.302	.046
V	.139	.056	.073	1.000	.347	.046	.195	.026
Cr	.109	.215	.001	.144	.123	.024	1.000	.181
Mn	.024	.230	.099	.062	.075	.024	.546	.667
Fe	.033	.217	.042	.059	.022	.141	.725	.152
Ni	.076	.115	.048	.904	.280	.044	.150	.044
Cu	.100	.157	.136	.049	.022	.116	.847	.142
Zn	.056	.069	.129	.001	.001	.044	.739	.032
Br	.089	.210	1.000	.059	.063	.025	.004	.093
Pb	.084	.155	.960	.048	.039	.002	.032	.116

Table A1. Continued

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.018	.788	.800	.036	.019	.327	.362	.023
EC	.015	.285	.156	.102	.022	.115	.155	.005
NO_3	.012	.655	.225	.247	.120	.475	.399	1.000
SO_4	.374	.217	.089	.281	1.000	.030	.139	.114
Na	.301	.143	.186	.364	.298	.086	.175	.008
Mg	.017	.094	.075	.057	.020	.226	.267	.052
Al	.077	.106	.088	.119	.046	1.000	.104	.043
Si	.007	.251	.036	.010	.001	.111	.054	.003
Cl	1.000	.166	.175	.406	.353	.164	.026	.012
K	.010	.653	.245	.091	.070	.320	.255	.475
Ca	.020	.450	.036	.035	.016	.211	.149	.022
Ti	.019	.556	.086	.036	.001	.282	.156	.009
V	.059	.054	.066	.849	.153	.046	.095	.007
Cr	.054	.376	.006	.279	.065	.032	.698	.087
Mn	.009	.315	.109	.100	.033	.031	.337	.318
Fe	.007	.183	.027	.034	.005	.144	.418	.063
Ni	.026	.081	.024	.487	.089	.023	.060	.020
Cu	.040	.203	.138	.053	.005	.140	.458	.054
Zn	.016	.059	.121	.011	.004	.053	.360	.021
Br	.038	.257	.952	.109	.031	.034	.005	.068
Pb	.014	.070	.336	.035	.008	.002	.012	.034

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.012	.284	.316	.018	.015	.222	.340	.035
EC	.010	.136	.091	.055	.013	.053	.093	.005
NO_3	.005	.388	.129	.265	.039	.298	.085	.000
SO_4	.026	.092	.038	.209	.000	.005	.058	.046
Na	.113	.058	.090	.279	.048	.025	.031	.007
Mg	.027	.138	.113	.051	.031	.299	.383	.076
Al	.036	.060	.061	.048	.017	.000	.048	.029
Si	.003	.038	.010	.007	.001	.039	.037	.001
Cl	.000	.058	.053	.316	.031	.036	.028	.009
K	.006	.402	.173	.056	.038	.143	.092	.147
Ca	.009	.144	.015	.023	.007	.047	.055	.009
Ti	.021	.343	.057	.033	.001	.275	.197	.009
V	.057	.057	.071	.262	.148	.036	.085	.006
Cr	.043	.314	.008	.379	.051	.040	.524	.065
Mn	.006	.231	.073	.121	.020	.029	.136	.106
Fe	.006	.150	.023	.028	.004	.162	.507	.079
Ni	.023	.086	.020	.481	.076	.019	.051	.019
Cu	.033	.168	.125	.067	.004	.097	.329	.037
Zn	.023	.092	.191	.010	.004	.074	.490	.028
Br	.023	.065	.083	.082	.020	.026	.004	.068
Pb	.012	.033	.125	.029	.007	.001	.010	.039

Table A1. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.155	.217	.000	.000	.006	.057	.000
EC	.001	.097	.040	.008	.001	.005	.071	.000
NO_3	.000	.084	.014	.005	.008	.013	.123	1.000
SO_4	.162	.021	.006	.016	1.000	.000	.026	.021
Na	.062	.006	.012	.019	.059	.001	.027	.000
Mg	.000	.007	.006	.007	.001	.026	.377	.018
Al	.047	.036	.032	.034	.016	1.000	.102	.018
Si	.002	.996	.027	.001	.000	.046	.105	.001
Cl	1.000	.011	.017	.028	.111	.003	.001	.000
K	.000	.154	.029	.003	.005	.012	.095	.425
Ca	.001	.187	.002	.001	.000	.011	.064	.002
Ti	.002	.916	.029	.001	.000	.039	.085	.001
V	.011	.003	.006	1.000	.061	.001	.039	.000
Cr	.004	.051	.000	.014	.005	.000	1.000	.021
Mn	.000	.043	.008	.002	.001	.000	.260	.307
Fe	.000	.048	.001	.001	.000	.005	.379	.011
Ni	.003	.015	.002	.639	.033	.000	.023	.002
Cu	.003	.019	.012	.001	.000	.004	.527	.010
Zn	.001	.002	.010	.001	.000	.001	.367	.001
Br	.002	.050	1.000	.003	.001	.000	.000	.007
Pb	.002	.025	.868	.002	.000	.000	.001	.011

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.023	.028	.000	.000	.001	.006	.000
EC	.000	.010	.013	.003	.001	.005	.016	.000
NO_3	.000	.023	.004	.002	.003	.004	.027	.000
SO_4	.018	.006	.004	.012	.000	.000	.013	.006
Na	.013	.002	.003	.010	.022	.000	.002	.000
Mg	.000	.001	.000	.001	.000	.011	.103	.004
Al	.006	.004	.009	.007	.006	.000	.023	.004
Si	.000	.007	.002	.000	.000	.005	.013	.001
Cl	.000	.003	.004	.012	.034	.002	.001	.000
K	.000	.030	.006	.002	.001	.003	.034	.116
Ca	.000	.012	.001	.001	.000	.002	.031	.001
Ti	.000	.079	.004	.001	.000	.001	.017	.001
V	.003	.001	.002	.000	.023	.000	.020	.000
Cr	.001	.013	.000	.002	.002	.000	.000	.004
Mn	.000	.009	.001	.001	.000	.000	.075	.081
Fe	.000	.013	.001	.001	.000	.002	.107	.004
Ni	.002	.003	.001	.107	.017	.000	.011	.000
Cu	.000	.001	.002	.001	.000	.001	.140	.003
Zn	.000	.001	.003	.001	.000	.000	.114	.000
Br	.001	.002	.000	.001	.001	.000	.000	.001
Pb	.001	.003	.056	.001	.000	.000	.001	.001

Table A1. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.025	.498	.637	.022	.023	.170	.251	.014
EC	.050	.476	.321	.159	.073	.173	.337	.019
NO_3	.015	.317	.139	.092	.139	.211	.319	1.000
SO_4	.410	.099	.053	.095	1.000	.013	.092	.091
Na	.527	.106	.170	.224	.497	.058	.196	.010
Mg	.040	.112	.109	.135	.054	.370	.685	.164
Al	.186	.111	.111	.126	.103	1.000	.154	.073
Si	.060	.969	.172	.032	.006	.362	.261	.022
Cl	1.000	.069	.093	.129	.321	.062	.014	.008
K	.017	.467	.214	.071	.116	.229	.300	.700
Ca	.064	.673	.067	.046	.047	.282	.314	.058
Ti	.061	.999	.191	.046	.004	.361	.253	.023
V	.121	.042	.067	.933	.283	.039	.126	.012
Cr	.103	.245	.005	.149	.111	.018	.905	.142
Mn	.017	.229	.108	.060	.058	.018	.464	.557
Fe	.027	.281	.051	.051	.016	.164	.658	.119
Ni	.085	.131	.052	1.000	.276	.041	.129	.044
Cu	.109	.205	.176	.037	.011	.155	.883	.135
Zn	.053	.076	.172	.033	.013	.077	.804	.052
Br	.062	.196	.934	.055	.046	.017	.004	.070
Pb	.065	.155	.980	.046	.030	.007	.031	.093

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.009	.067	.138	.007	.006	.050	.030	.012
EC	.013	.015	.026	.031	.022	.060	.032	.015
NO_3	.003	.047	.031	.014	.024	.033	.044	.000
SO_4	.014	.014	.016	.037	.000	.004	.026	.002
Na	.042	.012	.024	.035	.083	.002	.005	.007
Mg	.013	.010	.008	.009	.017	.050	.059	.021
Al	.021	.017	.024	.028	.007	.000	.028	.024
Si	.011	.048	.013	.006	.004	.049	.021	.008
Cl	.000	.005	.003	.024	.036	.013	.012	.003
K	.002	.073	.020	.036	.030	.058	.036	.083
Ca	.007	.011	.004	.018	.008	.034	.046	.012
Ti	.013	.002	.008	.003	.001	.054	.037	.007
V	.027	.015	.012	.044	.069	.006	.026	.006
Cr	.028	.045	.003	.030	.028	.011	.165	.017
Mn	.004	.010	.008	.005	.003	.007	.044	.087
Fe	.010	.011	.003	.018	.006	.016	.050	.014
Ni	.029	.020	.012	.000	.068	.008	.026	.008
Cu	.011	.033	.031	.029	.007	.026	.142	.028
Zn	.014	.019	.004	.038	.015	.017	.069	.019
Br	.020	.025	.115	.021	.018	.012	.002	.025
Pb	.021	.014	.026	.015	.014	.009	.005	.019

Table A1. Continued

MEANSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.181	.284	.000	.001	.024	.062	.000
EC	.002	.121	.055	.014	.005	.021	.081	.001
NO_3	.000	.059	.011	.005	.019	.031	.082	1.000
SO_4	.135	.006	.002	.006	1.000	.000	.007	.009
Na	.152	.005	.012	.023	.169	.002	.021	.000
Mg	.002	.008	.007	.012	.003	.104	.406	.029
Al	.038	.010	.010	.014	.015	1.000	.027	.007
Si	.005	.998	.031	.001	.000	.165	.097	.001
Cl	1.000	.004	.006	.013	.130	.004	.000	.000
K	.000	.151	.031	.004	.015	.042	.085	.571
Ca	.003	.240	.002	.001	.002	.050	.075	.003
Ti	.005	.940	.034	.002	.000	.145	.080	.001
V	.021	.002	.005	1.000	.147	.002	.025	.000
Cr	.012	.055	.000	.021	.018	.000	1.000	.031
Mn	.000	.044	.010	.003	.005	.000	.241	.427
Fe	.001	.058	.002	.002	.000	.023	.428	.018
Ni	.008	.013	.002	.764	.096	.001	.018	.002
Cu	.009	.023	.017	.001	.000	.016	.592	.017
Zn	.002	.003	.014	.001	.000	.004	.429	.002
Br	.006	.045	1.000	.004	.004	.000	.000	.009
Pb	.005	.023	.916	.002	.001	.000	.001	.014

STDSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.024	.029	.000	.000	.005	.004	.000
EC	.001	.012	.017	.005	.002	.015	.013	.000
NO_3	.000	.010	.003	.001	.004	.003	.020	.000
SO_4	.010	.002	.001	.005	.000	.000	.003	.002
Na	.026	.001	.002	.010	.045	.000	.001	.000
Mg	.001	.001	.000	.002	.001	.025	.094	.004
Al	.007	.001	.001	.003	.002	.000	.005	.003
Si	.001	.004	.002	.000	.000	.020	.008	.001
Cl	.000	.001	.001	.005	.028	.002	.000	.000
K	.000	.029	.006	.003	.004	.010	.021	.086
Ca	.001	.015	.001	.001	.001	.005	.032	.002
Ti	.001	.056	.003	.001	.000	.025	.010	.001
V	.007	.001	.002	.000	.055	.000	.012	.000
Cr	.002	.010	.000	.002	.004	.000	.000	.005
Mn	.000	.008	.002	.001	.001	.000	.051	.063
Fe	.000	.016	.001	.001	.000	.004	.096	.006
Ni	.005	.002	.001	.067	.046	.000	.008	.000
Cu	.001	.001	.002	.001	.000	.002	.119	.004
Zn	.001	.002	.003	.001	.000	.001	.103	.001
Br	.003	.002	.000	.002	.002	.000	.000	.002
Pb	.002	.002	.035	.001	.001	.000	.001	.002

Table A1. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.024	.424	.532	.019	.025	.154	.248	.015
EC	.042	.348	.233	.118	.068	.138	.285	.019
NO_3	.014	.243	.106	.072	.136	.176	.285	1.000
SO_4	.367	.078	.042	.076	1.000	.011	.082	.093
Na	.389	.068	.108	.148	.408	.041	.146	.008
Mg	.037	.089	.086	.110	.055	.321	.634	.169
Al	.195	.101	.100	.117	.122	1.000	.163	.084
Si	.070	.999	.175	.033	.008	.405	.311	.031
Cl	1.000	.060	.080	.115	.359	.059	.013	.009
K	.016	.387	.176	.059	.122	.204	.290	.755
Ca	.054	.490	.048	.034	.044	.223	.268	.056
Ti	.067	.969	.184	.046	.005	.380	.283	.031
V	.145	.043	.070	1.000	.379	.045	.155	.017
Cr	.111	.234	.005	.144	.135	.017	1.000	.177
Mn	.018	.208	.097	.056	.068	.018	.489	.652
Fe	.026	.240	.043	.044	.017	.152	.651	.132
Ni	.084	.111	.045	.874	.303	.038	.130	.049
Cu	.094	.153	.130	.029	.011	.126	.767	.130
Zn	.042	.053	.120	.023	.011	.059	.652	.045
Br	.076	.212	1.000	.059	.062	.020	.005	.095
Pb	.072	.152	.957	.046	.036	.008	.036	.118

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.004	.029	.027	.005	.004	.018	.007	.013
EC	.011	.017	.036	.022	.016	.051	.023	.015
NO_3	.004	.021	.016	.010	.013	.010	.036	.000
SO_4	.014	.016	.017	.032	.000	.004	.017	.013
Na	.032	.011	.012	.034	.057	.004	.002	.006
Mg	.015	.007	.003	.010	.015	.040	.072	.012
Al	.017	.007	.006	.014	.008	.000	.014	.017
Si	.010	.002	.005	.007	.006	.025	.013	.014
Cl	.000	.009	.008	.022	.038	.014	.011	.003
K	.002	.037	.016	.023	.017	.024	.036	.057
Ca	.006	.015	.007	.013	.007	.011	.063	.017
Ti	.012	.029	.007	.006	.001	.033	.017	.015
V	.022	.011	.015	.000	.069	.004	.038	.009
Cr	.008	.022	.004	.008	.016	.006	.000	.013
Mn	.006	.019	.009	.006	.009	.008	.050	.049
Fe	.008	.032	.007	.014	.005	.014	.074	.022
Ni	.028	.011	.015	.039	.073	.005	.033	.004
Cu	.005	.004	.007	.024	.009	.008	.077	.014
Zn	.012	.014	.013	.026	.013	.013	.077	.012
Br	.019	.004	.000	.014	.015	.011	.002	.010
Pb	.017	.007	.018	.013	.015	.011	.007	.008

Table A2. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 1

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.105	.527	.421	.033	.089	.209	.274	.035
EC	.076	.243	.104	.101	.087	.213	.154	.013
NO_3	.009	.159	.048	.032	.117	.258	.169	.838
SO_4	.201	.061	.023	.042	.836	.056	.078	.074
Na	.178	.063	.071	.072	.468	.138	.108	.006
Mg	.051	.055	.034	.104	.119	.371	.422	.224
Al	.260	.059	.036	.108	.212	1.000	.086	.130
Si	.055	.740	.062	.016	.005	.484	.172	.010
Cl	1.000	.100	.078	.085	.590	.279	.044	.015
K	.006	.264	.077	.033	.186	.240	.182	.639
Ca	.029	.170	.003	.014	.041	.109	.097	.024
Ti	.033	.637	.057	.017	.004	.448	.117	.009
V	.118	.055	.058	.818	.550	.149	.137	.004
Cr	.109	.275	.003	.103	.187	.001	.891	.234
Mn	.005	.172	.066	.037	.105	.060	.348	.741
Fe	.023	.151	.010	.024	.003	.123	.440	.124
Ni	.070	.134	.028	.712	.415	.098	.141	.080
Cu	.029	.055	.036	.004	.003	.123	.237	.056
Zn	.055	.016	.038	.028	.030	.032	.374	.051
Br	.203	.231	.910	.076	.181	.006	.020	.234
Pb	.091	.077	.500	.026	.053	.031	.017	.133

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.159	.410	.273	.048	.119	.063	.287	.051
EC	.121	.209	.087	.149	.128	.209	.178	.017
NO_3	.005	.110	.028	.008	.041	.255	.061	.142
SO_4	.122	.074	.026	.025	.284	.080	.062	.063
Na	.036	.061	.060	.025	.181	.168	.067	.004
Mg	.083	.046	.027	.154	.176	.282	.505	.302
Al	.358	.032	.017	.141	.240	.000	.075	.147
Si	.044	.254	.035	.011	.004	.288	.091	.003
Cl	.000	.109	.075	.041	.191	.367	.030	.008
K	.005	.197	.073	.021	.157	.191	.171	.388
Ca	.036	.043	.000	.016	.040	.048	.054	.021
Ti	.018	.373	.034	.004	.002	.404	.046	.004
V	.064	.045	.045	.315	.398	.156	.095	.003
Cr	.071	.186	.003	.040	.066	.001	.188	.038
Mn	.005	.103	.031	.024	.055	.060	.020	.271
Fe	.024	.102	.008	.024	.005	.095	.345	.103
Ni	.047	.066	.015	.268	.221	.079	.056	.006
Cu	.015	.036	.025	.001	.001	.109	.145	.018
Zn	.088	.020	.046	.046	.047	.032	.518	.079
Br	.265	.079	.155	.089	.186	.005	.010	.219
Pb	.088	.057	.448	.024	.044	.027	.014	.101

Table A2. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.078	.148	.000	.000	.002	.019	.000
EC	.000	.046	.030	.004	.001	.005	.021	.000
NO_3	.000	.044	.011	.004	.008	.008	.085	1.000
SO_4	.099	.008	.004	.011	1.000	.000	.032	.011
Na	.030	.003	.011	.014	.094	.001	.019	.000
Mg	.000	.003	.004	.004	.001	.021	.170	.013
Al	.040	.022	.023	.035	.024	1.000	.040	.031
Si	.002	1.000	.016	.001	.000	.042	.063	.000
Cl	1.000	.007	.012	.019	.159	.003	.003	.000
K	.000	.088	.016	.002	.007	.008	.040	.303
Ca	.000	.112	.000	.000	.001	.006	.040	.001
Ti	.001	.776	.016	.001	.000	.029	.041	.000
V	.007	.001	.004	1.000	.061	.001	.016	.000
Cr	.005	.055	.000	.015	.008	.000	1.000	.032
Mn	.000	.023	.010	.002	.002	.000	.155	.287
Fe	.000	.027	.000	.000	.000	.003	.194	.007
Ni	.001	.010	.001	.468	.023	.000	.016	.002
Cu	.001	.008	.008	.000	.000	.003	.220	.007
Zn	.000	.001	.007	.000	.000	.001	.159	.001
Br	.002	.022	.973	.002	.002	.000	.000	.008
Pb	.002	.009	.839	.001	.000	.000	.000	.011

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.001	.012	.000	.000	.000	.001	.000
EC	.000	.001	.002	.000	.000	.001	.001	.000
NO_3	.000	.004	.001	.000	.001	.001	.012	.000
SO_4	.010	.000	.000	.001	.000	.000	.003	.001
Na	.005	.000	.001	.001	.007	.000	.001	.000
Mg	.000	.000	.000	.000	.000	.001	.003	.001
Al	.003	.002	.001	.002	.002	.000	.002	.002
Si	.000	.000	.001	.000	.000	.002	.003	.000
Cl	.000	.000	.001	.002	.009	.000	.001	.000
K	.000	.002	.002	.000	.001	.001	.003	.004
Ca	.000	.003	.000	.000	.000	.000	.004	.000
Ti	.000	.075	.001	.000	.000	.001	.003	.000
V	.001	.000	.000	.000	.003	.000	.001	.000
Cr	.000	.000	.000	.002	.000	.000	.000	.005
Mn	.000	.002	.001	.000	.000	.000	.012	.047
Fe	.000	.001	.000	.000	.000	.000	.012	.001
Ni	.000	.000	.000	.062	.003	.000	.000	.000
Cu	.000	.001	.001	.000	.000	.000	.016	.002
Zn	.000	.000	.001	.000	.000	.000	.004	.000
Br	.000	.004	.046	.000	.000	.000	.000	.002
Pb	.000	.000	.160	.000	.000	.000	.000	.001

Table A2. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.032	.359	.509	.018	.025	.101	.161	.010
EC	.046	.268	.222	.092	.048	.148	.167	.010
NO_3	.014	.192	.100	.067	.122	.143	.244	1.000
SO_4	.350	.062	.043	.087	1.000	.024	.111	.079
Na	.283	.057	.106	.140	.453	.049	.127	.008
Mg	.027	.070	.079	.101	.067	.306	.478	.157
Al	.194	.088	.092	.133	.137	1.000	.109	.114
Si	.065	1.000	.132	.029	.004	.345	.230	.012
Cl	1.000	.051	.069	.100	.359	.057	.031	.010
K	.006	.336	.147	.059	.137	.168	.207	.685
Ca	.044	.409	.014	.032	.051	.153	.223	.039
Ti	.052	.821	.121	.036	.004	.269	.173	.011
V	.112	.032	.053	1.000	.306	.035	.095	.002
Cr	.121	.256	.004	.160	.147	.001	1.000	.213
Mn	.004	.159	.107	.050	.075	.025	.376	.612
Fe	.017	.183	.019	.030	.003	.096	.448	.098
Ni	.056	.101	.034	.849	.230	.035	.117	.055
Cu	.078	.112	.121	.017	.005	.114	.555	.117
Zn	.031	.028	.107	.027	.016	.047	.445	.040
Br	.074	.133	.906	.043	.056	.002	.012	.090
Pb	.078	.099	1.000	.036	.033	.024	.018	.123

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.007	.062	.075	.003	.007	.015	.025	.005
EC	.005	.016	.019	.008	.002	.027	.014	.004
NO_3	.001	.022	.008	.005	.017	.009	.015	.000
SO_4	.033	.005	.005	.012	.000	.006	.013	.012
Na	.027	.004	.006	.005	.044	.006	.005	.007
Mg	.008	.006	.007	.009	.015	.019	.065	.022
Al	.009	.003	.002	.008	.018	.000	.007	.002
Si	.001	.000	.009	.001	.000	.015	.005	.005
Cl	.000	.002	.001	.002	.037	.004	.002	.003
K	.001	.019	.015	.007	.004	.019	.020	.102
Ca	.000	.007	.004	.002	.005	.005	.005	.006
Ti	.003	.054	.001	.002	.001	.011	.008	.003
V	.011	.004	.002	.000	.049	.002	.007	.001
Cr	.003	.002	.003	.005	.015	.002	.000	.030
Mn	.001	.023	.014	.006	.018	.003	.055	.114
Fe	.001	.015	.004	.002	.002	.006	.028	.007
Ni	.009	.016	.006	.159	.056	.005	.020	.005
Cu	.010	.013	.012	.002	.001	.015	.061	.029
Zn	.002	.004	.005	.002	.002	.004	.022	.006
Br	.016	.026	.103	.007	.014	.003	.000	.022
Pb	.009	.012	.000	.003	.007	.003	.003	.016

Table A2. Continued

MEANSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.108	.220	.000	.001	.010	.026	.000
EC	.002	.067	.046	.007	.002	.024	.031	.000
NO_3	.000	.033	.009	.004	.015	.022	.064	1.000
SO_4	.130	.003	.002	.006	1.000	.001	.013	.006
Na	.093	.003	.011	.018	.225	.003	.019	.000
Mg	.001	.004	.005	.008	.004	.096	.231	.023
Al	.038	.006	.007	.014	.017	1.000	.012	.012
Si	.005	1.000	.018	.001	.000	.143	.064	.000
Cl	1.000	.002	.004	.008	.121	.003	.001	.000
K	.000	.103	.020	.003	.019	.031	.047	.471
Ca	.002	.163	.000	.001	.003	.028	.059	.002
Ti	.004	.850	.019	.002	.000	.110	.046	.000
V	.016	.001	.003	1.000	.108	.002	.011	.000
Cr	.015	.055	.000	.020	.020	.000	1.000	.042
Mn	.000	.025	.012	.002	.006	.001	.171	.420
Fe	.000	.038	.000	.001	.000	.013	.274	.012
Ni	.004	.010	.001	.654	.056	.001	.016	.003
Cu	.006	.011	.013	.000	.000	.013	.315	.013
Zn	.001	.001	.011	.001	.000	.003	.234	.002
Br	.008	.021	.985	.002	.004	.000	.000	.010
Pb	.006	.009	.898	.001	.001	.001	.000	.015

STDSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.002	.017	.000	.000	.001	.001	.000
EC	.000	.001	.004	.000	.000	.004	.002	.000
NO_3	.000	.003	.001	.000	.001	.001	.010	.000
SO_4	.006	.000	.000	.000	.000	.000	.001	.001
Na	.008	.000	.001	.001	.007	.000	.000	.000
Mg	.000	.000	.000	.000	.000	.003	.004	.002
Al	.001	.001	.000	.000	.001	.000	.000	.001
Si	.000	.000	.001	.000	.000	.006	.002	.000
Cl	.000	.000	.001	.001	.009	.000	.000	.000
K	.000	.003	.001	.000	.001	.002	.004	.005
Ca	.000	.002	.000	.000	.000	.001	.004	.000
Ti	.000	.053	.001	.000	.000	.007	.002	.000
V	.001	.000	.000	.000	.003	.000	.001	.000
Cr	.000	.001	.000	.001	.001	.000	.000	.006
Mn	.000	.001	.001	.000	.000	.000	.005	.041
Fe	.000	.002	.000	.000	.000	.000	.013	.002
Ni	.001	.000	.000	.045	.006	.000	.000	.000
Cu	.000	.001	.001	.000	.000	.001	.017	.002
Zn	.000	.000	.001	.000	.000	.000	.005	.001
Br	.001	.002	.027	.000	.000	.000	.000	.001
Pb	.000	.000	.103	.000	.000	.000	.000	.001

Table A2. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.032	.328	.469	.016	.024	.102	.162	.010
EC	.048	.258	.214	.087	.049	.155	.176	.010
NO_3	.014	.181	.095	.062	.122	.148	.253	1.000
SO_4	.360	.058	.041	.080	1.000	.024	.114	.078
Na	.305	.056	.104	.136	.474	.053	.137	.008
Mg	.026	.064	.073	.091	.065	.309	.480	.152
Al	.194	.080	.084	.119	.132	1.000	.108	.110
Si	.071	1.000	.132	.029	.005	.379	.252	.013
Cl	1.000	.046	.063	.090	.348	.057	.031	.010
K	.007	.321	.140	.055	.139	.175	.216	.687
Ca	.047	.404	.014	.031	.053	.167	.242	.041
Ti	.064	.921	.136	.040	.005	.332	.213	.013
V	.125	.032	.054	1.000	.329	.040	.106	.002
Cr	.121	.234	.004	.143	.142	.001	1.000	.205
Mn	.005	.160	.108	.049	.080	.028	.414	.647
Fe	.020	.195	.021	.031	.003	.113	.523	.111
Ni	.059	.098	.033	.808	.236	.038	.125	.057
Cu	.079	.103	.112	.015	.005	.115	.561	.113
Zn	.034	.027	.106	.026	.017	.051	.484	.042
Br	.087	.144	.992	.046	.064	.003	.014	.102
Pb	.080	.093	.947	.033	.033	.025	.018	.121

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.003	.003	.018	.001	.001	.003	.003	.003
EC	.002	.001	.009	.002	.003	.012	.005	.003
NO_3	.000	.008	.006	.003	.004	.003	.019	.000
SO_4	.009	.001	.002	.002	.000	.003	.005	.004
Na	.014	.002	.004	.004	.008	.003	.001	.006
Mg	.004	.003	.001	.001	.001	.005	.004	.006
Al	.003	.004	.003	.001	.006	.000	.002	.005
Si	.001	.000	.002	.002	.001	.009	.005	.006
Cl	.000	.002	.005	.005	.013	.001	.003	.002
K	.001	.005	.005	.003	.004	.005	.009	.004
Ca	.001	.003	.003	.001	.002	.003	.009	.003
Ti	.001	.029	.004	.002	.000	.010	.004	.005
V	.003	.002	.002	.000	.005	.001	.003	.001
Cr	.001	.002	.002	.005	.002	.002	.000	.016
Mn	.001	.002	.006	.002	.000	.002	.006	.032
Fe	.000	.004	.002	.001	.002	.002	.012	.009
Ni	.005	.002	.003	.028	.013	.000	.002	.002
Cu	.002	.005	.007	.001	.002	.004	.015	.011
Zn	.001	.003	.006	.001	.002	.001	.005	.008
Br	.004	.008	.014	.003	.002	.003	.002	.007
Pb	.002	.002	.054	.002	.001	.002	.001	.003

Table A3. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 2

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.031	.345	.301	.009	.022	.112	.131	.014
EC	.029	.311	.093	.062	.064	.089	.162	.014
NO_3	.009	.179	.030	.021	.085	.037	.137	.529
SO_4	.248	.068	.022	.045	.775	.011	.046	.066
Na	.170	.050	.037	.045	.249	.013	.066	.007
Mg	.030	.159	.087	.108	.112	.469	.792	.329
Al	.398	.241	.103	.102	.303	.679	.232	.203
Si	.074	.605	.072	.012	.006	.288	.127	.020
Cl	.800	.095	.043	.093	.517	.046	.035	.013
K	.018	.277	.075	.017	.073	.071	.128	.543
Ca	.060	.439	.020	.017	.039	.152	.166	.052
Ti	.089	.875	.098	.020	.002	.240	.167	.023
V	.419	.093	.104	1.000	.764	.053	.202	.011
Cr	.146	.214	.002	.050	.104	.004	.650	.202
Mn	.014	.298	.064	.042	.090	.006	.503	.797
Fe	.023	.285	.024	.025	.013	.134	.530	.158
Ni	.146	.160	.044	.493	.384	.031	.143	.090
Cu	.102	.133	.074	.014	.002	.147	.498	.153
Zn	.053	.060	.085	.024	.020	.071	.609	.074
Br	.071	.220	.485	.031	.080	.004	.013	.092
Pb	.149	.266	1.000	.052	.097	.015	.037	.244

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.034	.078	.255	.009	.008	.113	.031	.017
EC	.007	.213	.029	.055	.044	.098	.111	.021
NO_3	.008	.239	.023	.026	.105	.017	.176	.447
SO_4	.099	.045	.004	.029	.374	.008	.023	.018
Na	.174	.055	.029	.047	.240	.006	.071	.005
Mg	.014	.071	.043	.073	.030	.464	.262	.123
Al	.423	.289	.093	.122	.343	.556	.282	.175
Si	.071	.455	.065	.013	.005	.344	.097	.017
Cl	.346	.106	.029	.082	.472	.041	.041	.008
K	.024	.189	.078	.009	.038	.037	.081	.419
Ca	.059	.033	.016	.008	.009	.132	.029	.028
Ti	.097	.217	.091	.005	.003	.173	.039	.009
V	.503	.047	.108	.000	.246	.029	.089	.009
Cr	.202	.148	.002	.023	.069	.003	.457	.230
Mn	.005	.261	.011	.030	.055	.004	.443	.290
Fe	.010	.062	.013	.016	.006	.130	.184	.057
Ni	.192	.119	.050	.295	.268	.029	.107	.097
Cu	.080	.116	.055	.017	.002	.209	.435	.143
Zn	.032	.041	.037	.025	.019	.088	.330	.060
Br	.046	.283	.357	.038	.100	.004	.019	.075
Pb	.038	.180	.000	.034	.068	.004	.022	.051

Table A3. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.115	.153	.000	.000	.004	.031	.000
EC	.001	.081	.035	.006	.001	.005	.041	.000
NO_3	.000	.072	.013	.004	.010	.012	.093	1.000
SO_4	.122	.017	.008	.018	1.000	.001	.017	.014
Na	.039	.006	.014	.021	.093	.001	.023	.000
Mg	.000	.005	.005	.006	.001	.026	.256	.015
Al	.048	.032	.022	.029	.028	1.000	.056	.024
Si	.002	1.000	.019	.001	.000	.048	.080	.000
Cl	1.000	.011	.017	.028	.158	.004	.003	.000
K	.000	.133	.021	.002	.005	.012	.057	.353
Ca	.001	.161	.001	.001	.000	.009	.043	.001
Ti	.002	.853	.020	.001	.000	.038	.059	.000
V	.010	.002	.006	1.000	.079	.001	.023	.000
Cr	.005	.059	.000	.014	.007	.000	1.000	.025
Mn	.000	.034	.009	.002	.002	.000	.186	.272
Fe	.000	.041	.001	.001	.000	.004	.253	.008
Ni	.002	.012	.002	.515	.035	.001	.017	.002
Cu	.002	.011	.009	.000	.000	.003	.292	.007
Zn	.000	.001	.009	.000	.000	.001	.247	.001
Br	.003	.032	.916	.002	.002	.000	.000	.007
Pb	.003	.015	.917	.001	.001	.000	.001	.012

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.024	.008	.000	.000	.001	.004	.000
EC	.000	.012	.005	.002	.001	.003	.002	.000
NO_3	.000	.009	.004	.001	.003	.002	.006	.000
SO_4	.017	.003	.003	.008	.000	.000	.004	.001
Na	.009	.001	.002	.009	.021	.001	.001	.000
Mg	.000	.001	.001	.002	.000	.005	.034	.002
Al	.003	.006	.003	.003	.006	.000	.007	.002
Si	.000	.000	.002	.000	.000	.002	.008	.000
Cl	.000	.002	.003	.011	.029	.001	.001	.000
K	.000	.027	.002	.001	.000	.002	.008	.015
Ca	.000	.034	.000	.000	.000	.002	.010	.000
Ti	.000	.039	.002	.001	.000	.002	.003	.000
V	.002	.001	.001	.000	.007	.000	.001	.000
Cr	.000	.005	.000	.003	.001	.000	.000	.007
Mn	.000	.005	.002	.000	.000	.000	.008	.057
Fe	.000	.009	.000	.000	.000	.000	.057	.001
Ni	.001	.002	.001	.181	.014	.000	.001	.000
Cu	.000	.001	.002	.000	.000	.001	.019	.002
Zn	.000	.001	.001	.000	.000	.000	.021	.000
Br	.000	.010	.145	.000	.000	.000	.000	.002
Pb	.001	.001	.109	.001	.001	.000	.000	.001

Table A3. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.028	.479	.573	.021	.026	.159	.257	.015
EC	.054	.430	.293	.138	.081	.175	.320	.013
NO_3	.018	.250	.108	.072	.132	.175	.296	1.000
SO_4	.363	.091	.062	.110	1.000	.024	.093	.089
Na	.353	.095	.146	.205	.523	.065	.188	.015
Mg	.020	.103	.102	.128	.071	.390	.756	.188
Al	.194	.105	.090	.120	.142	1.000	.145	.098
Si	.070	.985	.141	.032	.006	.373	.289	.022
Cl	1.000	.071	.090	.131	.379	.066	.038	.012
K	.019	.459	.186	.067	.124	.235	.313	.800
Ca	.053	.590	.038	.042	.047	.244	.314	.055
Ti	.065	.943	.148	.044	.003	.346	.257	.022
V	.125	.040	.064	.984	.334	.037	.130	.004
Cr	.099	.234	.003	.138	.115	.010	1.000	.163
Mn	.014	.219	.114	.060	.068	.014	.538	.665
Fe	.021	.267	.037	.040	.011	.151	.679	.124
Ni	.075	.119	.045	.922	.285	.045	.149	.052
Cu	.093	.150	.137	.024	.002	.136	.799	.127
Zn	.044	.046	.138	.032	.013	.068	.737	.053
Br	.085	.179	1.000	.057	.065	.012	.010	.092
Pb	.071	.108	.871	.039	.037	.014	.021	.102

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.007	.086	.039	.007	.004	.046	.032	.011
EC	.017	.023	.033	.014	.026	.033	.044	.016
NO_3	.006	.024	.012	.002	.025	.015	.041	.000
SO_4	.007	.012	.010	.002	.000	.006	.017	.005
Na	.019	.008	.008	.008	.074	.012	.018	.005
Mg	.007	.020	.023	.018	.020	.051	.169	.024
Al	.041	.013	.015	.012	.040	.000	.027	.018
Si	.013	.026	.010	.002	.002	.046	.029	.007
Cl	.000	.014	.008	.006	.017	.003	.013	.003
K	.006	.098	.018	.006	.005	.043	.065	.071
Ca	.007	.114	.010	.006	.003	.045	.053	.007
Ti	.009	.055	.021	.003	.004	.075	.004	.007
V	.028	.006	.011	.027	.077	.002	.026	.000
Cr	.014	.024	.001	.021	.016	.011	.000	.031
Mn	.004	.008	.010	.002	.003	.011	.087	.018
Fe	.006	.061	.006	.003	.004	.029	.071	.016
Ni	.013	.025	.008	.083	.040	.012	.035	.008
Cu	.008	.005	.008	.002	.001	.015	.062	.017
Zn	.008	.016	.020	.009	.005	.013	.051	.018
Br	.015	.024	.000	.003	.015	.013	.007	.011
Pb	.011	.012	.070	.001	.012	.007	.006	.001

Table A3. Continued

MEANSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.146	.220	.000	.001	.018	.039	.000
EC	.002	.105	.051	.011	.005	.021	.053	.000
NO_3	.000	.051	.010	.004	.019	.029	.065	1.000
SO_4	.137	.006	.003	.009	1.000	.001	.006	.007
Na	.108	.005	.014	.026	.224	.003	.019	.000
Mg	.000	.006	.006	.010	.004	.105	.308	.026
Al	.045	.010	.007	.012	.023	1.000	.016	.010
Si	.007	1.000	.022	.001	.000	.163	.078	.001
Cl	1.000	.004	.006	.012	.138	.004	.001	.000
K	.000	.139	.024	.003	.014	.041	.059	.519
Ca	.003	.215	.001	.001	.002	.042	.056	.002
Ti	.006	.899	.023	.002	.000	.136	.061	.001
V	.022	.002	.004	1.000	.153	.002	.016	.000
Cr	.015	.059	.000	.020	.019	.000	1.000	.035
Mn	.000	.036	.010	.003	.005	.000	.193	.402
Fe	.000	.053	.001	.001	.000	.019	.320	.014
Ni	.006	.011	.002	.678	.089	.002	.016	.003
Cu	.008	.015	.013	.000	.000	.014	.380	.013
Zn	.002	.001	.013	.001	.000	.003	.324	.002
Br	.009	.029	.948	.003	.005	.000	.000	.009
Pb	.009	.014	.948	.002	.002	.000	.001	.015

STDSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.027	.011	.000	.000	.005	.005	.000
EC	.001	.013	.008	.003	.002	.009	.001	.000
NO_3	.000	.005	.003	.001	.004	.003	.006	.000
SO_4	.003	.001	.001	.004	.000	.000	.001	.001
Na	.020	.000	.002	.007	.034	.002	.001	.000
Mg	.000	.001	.001	.002	.001	.010	.034	.002
Al	.007	.001	.002	.001	.006	.000	.001	.002
Si	.001	.000	.003	.000	.000	.015	.005	.000
Cl	.000	.001	.001	.003	.009	.001	.000	.000
K	.000	.026	.002	.001	.000	.005	.010	.017
Ca	.000	.038	.001	.000	.000	.009	.012	.000
Ti	.001	.026	.002	.001	.000	.015	.002	.000
V	.003	.000	.001	.000	.014	.000	.002	.000
Cr	.001	.003	.000	.003	.001	.000	.000	.008
Mn	.000	.003	.002	.000	.001	.000	.010	.056
Fe	.000	.011	.000	.001	.000	.003	.061	.002
Ni	.002	.002	.001	.128	.025	.000	.002	.000
Cu	.001	.001	.003	.000	.000	.002	.023	.004
Zn	.000	.001	.002	.000	.000	.001	.021	.001
Br	.001	.007	.090	.000	.001	.000	.000	.002
Pb	.002	.002	.069	.001	.001	.000	.000	.002

Table A3. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.026	.381	.469	.017	.025	.133	.196	.014
EC	.047	.324	.226	.104	.070	.142	.229	.011
NO_3	.019	.226	.101	.066	.138	.169	.255	1.000
SO_4	.371	.078	.055	.095	1.000	.023	.076	.084
Na	.327	.074	.117	.160	.472	.055	.139	.013
Mg	.018	.079	.080	.099	.063	.324	.554	.161
Al	.213	.097	.085	.111	.152	1.000	.128	.100
Si	.084	1.000	.147	.033	.007	.403	.280	.025
Cl	1.000	.059	.077	.110	.371	.060	.030	.011
K	.019	.372	.156	.055	.119	.203	.242	.721
Ca	.050	.463	.031	.033	.043	.205	.236	.047
Ti	.078	.948	.152	.044	.003	.368	.247	.025
V	.149	.041	.066	1.000	.390	.040	.125	.004
Cr	.122	.244	.003	.143	.139	.010	1.000	.187
Mn	.015	.189	.101	.051	.069	.013	.439	.633
Fe	.022	.229	.032	.035	.011	.139	.564	.118
Ni	.079	.105	.041	.821	.297	.042	.125	.051
Cu	.089	.121	.113	.020	.002	.117	.616	.113
Zn	.042	.037	.113	.025	.012	.058	.569	.047
Br	.095	.170	.973	.054	.071	.011	.008	.096
Pb	.092	.118	.973	.043	.047	.017	.023	.123

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.006	.036	.011	.005	.003	.021	.012	.010
EC	.011	.020	.017	.014	.013	.032	.003	.013
NO_3	.006	.010	.014	.007	.014	.010	.012	.000
SO_4	.003	.004	.012	.018	.000	.010	.010	.006
Na	.030	.003	.008	.023	.036	.015	.003	.005
Mg	.005	.009	.008	.010	.007	.016	.031	.007
Al	.016	.006	.010	.005	.020	.000	.004	.012
Si	.008	.000	.009	.005	.003	.019	.009	.007
Cl	.000	.007	.008	.012	.013	.008	.007	.003
K	.005	.035	.007	.007	.002	.012	.021	.012
Ca	.005	.042	.009	.000	.002	.022	.026	.003
Ti	.007	.014	.008	.006	.004	.020	.003	.006
V	.008	.004	.005	.000	.018	.002	.008	.000
Cr	.005	.006	.001	.011	.004	.010	.000	.022
Mn	.004	.009	.011	.004	.006	.010	.011	.045
Fe	.007	.025	.004	.008	.004	.009	.055	.007
Ni	.015	.009	.009	.079	.041	.006	.008	.003
Cu	.007	.003	.013	.004	.002	.010	.018	.017
Zn	.004	.013	.009	.002	.003	.007	.018	.010
Br	.007	.021	.047	.004	.008	.012	.006	.010
Pb	.013	.007	.036	.008	.014	.011	.008	.007

Table A4. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 3

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.018	.788	.800	.036	.019	.327	.362	.023
EC	.015	.285	.156	.102	.022	.115	.155	.005
NO_3	.012	.655	.225	.247	.120	.475	.399	1.000
SO_4	.374	.217	.089	.281	1.000	.030	.139	.114
Na	.301	.143	.186	.364	.298	.086	.175	.008
Mg	.017	.094	.075	.057	.020	.226	.267	.052
Al	.077	.106	.088	.119	.046	1.000	.104	.043
Si	.007	.251	.036	.010	.001	.111	.054	.003
Cl	1.000	.166	.175	.406	.353	.164	.026	.012
K	.010	.653	.245	.091	.070	.320	.255	.475
Ca	.020	.450	.036	.035	.016	.211	.149	.022
Ti	.019	.556	.086	.036	.001	.282	.156	.009
V	.059	.054	.066	.849	.153	.046	.095	.007
Cr	.054	.376	.006	.279	.065	.032	.698	.087
Mn	.009	.315	.109	.100	.033	.031	.337	.318
Fe	.007	.183	.027	.034	.005	.144	.418	.063
Ni	.026	.081	.024	.487	.089	.023	.060	.020
Cu	.040	.203	.138	.053	.005	.140	.458	.054
Zn	.016	.059	.121	.011	.004	.053	.360	.021
Br	.038	.257	.952	.109	.031	.034	.005	.068
Pb	.014	.070	.336	.035	.008	.002	.012	.034

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.012	.284	.316	.018	.015	.222	.340	.035
EC	.010	.136	.091	.055	.013	.053	.093	.005
NO_3	.005	.388	.129	.265	.039	.298	.085	.000
SO_4	.026	.092	.038	.209	.000	.005	.058	.046
Na	.113	.058	.090	.279	.048	.025	.031	.007
Mg	.027	.138	.113	.051	.031	.299	.383	.076
Al	.036	.060	.061	.048	.017	.000	.048	.029
Si	.003	.038	.010	.007	.001	.039	.037	.001
Cl	.000	.058	.053	.316	.031	.036	.028	.009
K	.006	.402	.173	.056	.038	.143	.092	.147
Ca	.009	.144	.015	.023	.007	.047	.055	.009
Ti	.021	.343	.057	.033	.001	.275	.197	.009
V	.057	.057	.071	.262	.148	.036	.085	.006
Cr	.043	.314	.008	.379	.051	.040	.524	.065
Mn	.006	.231	.073	.121	.020	.029	.136	.106
Fe	.006	.150	.023	.028	.004	.162	.507	.079
Ni	.023	.086	.020	.481	.076	.019	.051	.019
Cu	.033	.168	.125	.067	.004	.097	.329	.037
Zn	.023	.092	.191	.010	.004	.074	.490	.028
Br	.023	.065	.083	.082	.020	.026	.004	.068
Pb	.012	.033	.125	.029	.007	.001	.010	.039

Table A4. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.155	.217	.000	.000	.006	.057	.000
EC	.001	.097	.040	.008	.001	.005	.071	.000
NO_3	.000	.084	.014	.005	.008	.013	.123	1.000
SO_4	.162	.021	.006	.016	1.000	.000	.026	.021
Na	.062	.006	.012	.019	.059	.001	.027	.000
Mg	.000	.007	.006	.007	.001	.026	.377	.018
Al	.047	.036	.032	.034	.016	1.000	.102	.018
Si	.002	.996	.027	.001	.000	.046	.105	.001
Cl	1.000	.011	.017	.028	.111	.003	.001	.000
K	.000	.154	.029	.003	.005	.012	.095	.425
Ca	.001	.187	.002	.001	.000	.011	.064	.002
Ti	.002	.916	.029	.001	.000	.039	.085	.001
V	.011	.003	.006	1.000	.061	.001	.039	.000
Cr	.004	.051	.000	.014	.005	.000	1.000	.021
Mn	.000	.043	.008	.002	.001	.000	.260	.307
Fe	.000	.048	.001	.001	.000	.005	.379	.011
Ni	.003	.015	.002	.639	.033	.000	.023	.002
Cu	.003	.019	.012	.001	.000	.004	.527	.010
Zn	.001	.002	.010	.001	.000	.001	.367	.001
Br	.002	.050	1.000	.003	.001	.000	.000	.007
Pb	.002	.025	.868	.002	.000	.000	.001	.011

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.023	.028	.000	.000	.001	.006	.000
EC	.000	.010	.013	.003	.001	.005	.016	.000
NO_3	.000	.023	.004	.002	.003	.004	.027	.000
SO_4	.018	.006	.004	.012	.000	.000	.013	.006
Na	.013	.002	.003	.010	.022	.000	.002	.000
Mg	.000	.001	.000	.001	.000	.011	.103	.004
Al	.006	.004	.009	.007	.006	.000	.023	.004
Si	.000	.007	.002	.000	.000	.005	.013	.001
Cl	.000	.003	.004	.012	.034	.002	.001	.000
K	.000	.030	.006	.002	.001	.003	.034	.116
Ca	.000	.012	.001	.001	.000	.002	.031	.001
Ti	.000	.079	.004	.001	.000	.001	.017	.001
V	.003	.001	.002	.000	.023	.000	.020	.000
Cr	.001	.013	.000	.002	.002	.000	.000	.004
Mn	.000	.009	.001	.001	.000	.000	.075	.081
Fe	.000	.013	.001	.001	.000	.002	.107	.004
Ni	.002	.003	.001	.107	.017	.000	.011	.000
Cu	.000	.001	.002	.001	.000	.001	.140	.003
Zn	.000	.001	.003	.001	.000	.000	.114	.000
Br	.001	.002	.000	.001	.001	.000	.000	.001
Pb	.001	.003	.056	.001	.000	.000	.001	.001

Table A4. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.025	.498	.637	.022	.023	.170	.251	.014
EC	.050	.476	.321	.159	.073	.173	.337	.019
NO_3	.015	.317	.139	.092	.139	.211	.319	1.000
SO_4	.410	.099	.053	.095	1.000	.013	.092	.091
Na	.527	.106	.170	.224	.497	.058	.196	.010
Mg	.040	.112	.109	.135	.054	.370	.685	.164
Al	.186	.111	.111	.126	.103	1.000	.154	.073
Si	.060	.969	.172	.032	.006	.362	.261	.022
Cl	1.000	.069	.093	.129	.321	.062	.014	.008
K	.017	.467	.214	.071	.116	.229	.300	.700
Ca	.064	.673	.067	.046	.047	.282	.314	.058
Ti	.061	.999	.191	.046	.004	.361	.253	.023
V	.121	.042	.067	.933	.283	.039	.126	.012
Cr	.103	.245	.005	.149	.111	.018	.905	.142
Mn	.017	.229	.108	.060	.058	.018	.464	.557
Fe	.027	.281	.051	.051	.016	.164	.658	.119
Ni	.085	.131	.052	1.000	.276	.041	.129	.044
Cu	.109	.205	.176	.037	.011	.155	.883	.135
Zn	.053	.076	.172	.033	.013	.077	.804	.052
Br	.062	.196	.934	.055	.046	.017	.004	.070
Pb	.065	.155	.980	.046	.030	.007	.031	.093

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.009	.067	.138	.007	.006	.050	.030	.012
EC	.013	.015	.026	.031	.022	.060	.032	.015
NO_3	.003	.047	.031	.014	.024	.033	.044	.000
SO_4	.014	.014	.016	.037	.000	.004	.026	.002
Na	.042	.012	.024	.035	.083	.002	.005	.007
Mg	.013	.010	.008	.009	.017	.050	.059	.021
Al	.021	.017	.024	.028	.007	.000	.028	.024
Si	.011	.048	.013	.006	.004	.049	.021	.008
Cl	.000	.005	.003	.024	.036	.013	.012	.003
K	.002	.073	.020	.036	.030	.058	.036	.083
Ca	.007	.011	.004	.018	.008	.034	.046	.012
Ti	.013	.002	.008	.003	.001	.054	.037	.007
V	.027	.015	.012	.044	.069	.006	.026	.006
Cr	.028	.045	.003	.030	.028	.011	.165	.017
Mn	.004	.010	.008	.005	.003	.007	.044	.087
Fe	.010	.011	.003	.018	.006	.016	.050	.014
Ni	.029	.020	.012	.000	.068	.008	.026	.008
Cu	.011	.033	.031	.029	.007	.026	.142	.028
Zn	.014	.019	.004	.038	.015	.017	.069	.019
Br	.020	.025	.115	.021	.018	.012	.002	.025
Pb	.021	.014	.026	.015	.014	.009	.005	.019

Table A4. Continued

MEANSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.001	.181	.284	.000	.001	.024	.062	.000
EC	.002	.121	.055	.014	.005	.021	.081	.001
NO_3	.000	.059	.011	.005	.019	.031	.082	1.000
SO_4	.135	.006	.002	.006	1.000	.000	.007	.009
Na	.152	.005	.012	.023	.169	.002	.021	.000
Mg	.002	.008	.007	.012	.003	.104	.406	.029
Al	.038	.010	.010	.014	.015	1.000	.027	.007
Si	.005	.998	.031	.001	.000	.165	.097	.001
Cl	1.000	.004	.006	.013	.130	.004	.000	.000
K	.000	.151	.031	.004	.015	.042	.085	.571
Ca	.003	.240	.002	.001	.002	.050	.075	.003
Ti	.005	.940	.034	.002	.000	.145	.080	.001
V	.021	.002	.005	1.000	.147	.002	.025	.000
Cr	.012	.055	.000	.021	.018	.000	1.000	.031
Mn	.000	.044	.010	.003	.005	.000	.241	.427
Fe	.001	.058	.002	.002	.000	.023	.428	.018
Ni	.008	.013	.002	.764	.096	.001	.018	.002
Cu	.009	.023	.017	.001	.000	.016	.592	.017
Zn	.002	.003	.014	.001	.000	.004	.429	.002
Br	.006	.045	1.000	.004	.004	.000	.000	.009
Pb	.005	.023	.916	.002	.001	.000	.001	.014

STDSPINSBETA

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.000	.024	.029	.000	.000	.005	.004	.000
EC	.001	.012	.017	.005	.002	.015	.013	.000
NO_3	.000	.010	.003	.001	.004	.003	.020	.000
SO_4	.010	.002	.001	.005	.000	.000	.003	.002
Na	.026	.001	.002	.010	.045	.000	.001	.000
Mg	.001	.001	.000	.002	.001	.025	.094	.004
Al	.007	.001	.001	.003	.002	.000	.005	.003
Si	.001	.004	.002	.000	.000	.020	.008	.001
Cl	.000	.001	.001	.005	.028	.002	.000	.000
K	.000	.029	.006	.003	.004	.010	.021	.086
Ca	.001	.015	.001	.001	.001	.005	.032	.002
Ti	.001	.056	.003	.001	.000	.025	.010	.001
V	.007	.001	.002	.000	.055	.000	.012	.000
Cr	.002	.010	.000	.002	.004	.000	.000	.005
Mn	.000	.008	.002	.001	.001	.000	.051	.063
Fe	.000	.016	.001	.001	.000	.004	.096	.006
Ni	.005	.002	.001	.067	.046	.000	.008	.000
Cu	.001	.001	.002	.001	.000	.002	.119	.004
Zn	.001	.002	.003	.001	.000	.001	.103	.001
Br	.003	.002	.000	.002	.002	.000	.000	.002
Pb	.002	.002	.035	.001	.001	.000	.001	.002

Table A4. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.024	.424	.532	.019	.025	.154	.248	.015
EC	.042	.348	.233	.118	.068	.138	.285	.019
NO_3	.014	.243	.106	.072	.136	.176	.285	1.000
SO_4	.367	.078	.042	.076	1.000	.011	.082	.093
Na	.389	.068	.108	.148	.408	.041	.146	.008
Mg	.037	.089	.086	.110	.055	.321	.634	.169
Al	.195	.101	.100	.117	.122	1.000	.163	.084
Si	.070	.999	.175	.033	.008	.405	.311	.031
Cl	1.000	.060	.080	.115	.359	.059	.013	.009
K	.016	.387	.176	.059	.122	.204	.290	.755
Ca	.054	.490	.048	.034	.044	.223	.268	.056
Ti	.067	.969	.184	.046	.005	.380	.283	.031
V	.145	.043	.070	1.000	.379	.045	.155	.017
Cr	.111	.234	.005	.144	.135	.017	1.000	.177
Mn	.018	.208	.097	.056	.068	.018	.489	.652
Fe	.026	.240	.043	.044	.017	.152	.651	.132
Ni	.084	.111	.045	.874	.303	.038	.130	.049
Cu	.094	.153	.130	.029	.011	.126	.767	.130
Zn	.042	.053	.120	.023	.011	.059	.652	.045
Br	.076	.212	1.000	.059	.062	.020	.005	.095
Pb	.072	.152	.957	.046	.036	.008	.036	.118

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL	KRAFT	ALPRO	STEEL	FeMn
OC	.004	.029	.027	.005	.004	.018	.007	.013
EC	.011	.017	.036	.022	.016	.051	.023	.015
NO_3	.004	.021	.016	.010	.013	.010	.036	.000
SO_4	.014	.016	.017	.032	.000	.004	.017	.013
Na	.032	.011	.012	.034	.057	.004	.002	.006
Mg	.015	.007	.003	.010	.015	.040	.072	.012
Al	.017	.007	.006	.014	.008	.000	.014	.017
Si	.010	.002	.005	.007	.006	.025	.013	.014
Cl	.000	.009	.008	.022	.038	.014	.011	.003
K	.002	.037	.016	.023	.017	.024	.036	.057
Ca	.006	.015	.007	.013	.007	.011	.063	.017
Ti	.012	.029	.007	.006	.001	.033	.017	.015
V	.022	.011	.015	.000	.069	.004	.038	.009
Cr	.008	.022	.004	.008	.016	.006	.000	.013
Mn	.006	.019	.009	.006	.009	.008	.050	.049
Fe	.008	.032	.007	.014	.005	.014	.074	.022
Ni	.028	.011	.015	.039	.073	.005	.033	.004
Cu	.005	.004	.007	.024	.009	.008	.077	.014
Zn	.012	.014	.013	.026	.013	.013	.077	.012
Br	.019	.004	.000	.014	.015	.011	.002	.010
Pb	.017	.007	.018	.013	.015	.011	.007	.008

Table A5. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 4

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.117	.079	.365	.029
EC	.055	.168	.243	.022
NO_3	.077	.087	.683	.080
SO_4	.057	.095	.102	.446
Na	.642	.040	.158	.022
Mg	.271	.368	.182	.041
Al	.022	.282	.036	.015
Si	.151	.489	.134	.051
Cl	1.000	.220	.257	.056
K	.055	.694	.192	.026
Ca	.034	.320	.017	.000
Ti	.085	.628	.196	.030
V	.073	.068	.195	.527
Cr	.192	.430	.163	.061
Mn	.064	.380	.128	.008
Fe	.090	.449	.025	.007
Ni	.089	.165	.316	.877
Cu	.021	.069	.085	.017
Zn	.115	.208	.558	.115
Br	.047	.069	.688	.039
Pb	.057	.068	.624	.041

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.193	.108	.552	.046
EC	.043	.063	.141	.004
NO_3	.099	.039	.446	.070
SO_4	.054	.112	.083	.481
Na	.307	.027	.103	.006
Mg	.312	.342	.194	.031
Al	.025	.387	.038	.019
Si	.228	.309	.108	.059
Cl	.000	.163	.257	.029
K	.015	.482	.159	.011
Ca	.044	.205	.013	.000
Ti	.068	.341	.163	.010
V	.102	.058	.184	.488
Cr	.315	.495	.209	.090
Mn	.065	.196	.103	.004
Fe	.092	.122	.016	.003
Ni	.083	.075	.250	.213
Cu	.019	.102	.108	.020
Zn	.094	.089	.157	.031
Br	.048	.001	.269	.021
Pb	.045	.067	.344	.029

Table A5. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.002	.089	.173	.003
EC	.001	.198	.044	.002
NO_3	.002	.084	.434	.027
SO_4	.002	.033	.007	.611
Na	.363	.011	.023	.003
Mg	.017	.634	.011	.004
Al	.001	.905	.004	.003
Si	.001	.988	.007	.003
Cl	1.000	.279	.039	.016
K	.001	.736	.006	.001
Ca	.000	.540	.000	.000
Ti	.001	.952	.008	.002
V	.001	.035	.020	.945
Cr	.001	.727	.009	.003
Mn	.001	.895	.009	.000
Fe	.001	.700	.000	.000
Ni	.001	.050	.016	.910
Cu	.001	.139	.051	.007
Zn	.002	.079	.070	.016
Br	.002	.101	1.000	.015
Pb	.002	.049	.764	.012

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.000	.012	.005	.000
EC	.000	.015	.005	.000
NO_3	.000	.011	.047	.003
SO_4	.000	.006	.001	.025
Na	.111	.003	.001	.001
Mg	.003	.099	.001	.001
Al	.000	.090	.000	.000
Si	.000	.021	.001	.000
Cl	.000	.046	.002	.001
K	.000	.105	.000	.000
Ca	.000	.082	.000	.000
Ti	.000	.072	.001	.000
V	.000	.006	.003	.095
Cr	.000	.061	.001	.000
Mn	.000	.094	.000	.000
Fe	.000	.037	.000	.000
Ni	.000	.008	.001	.084
Cu	.000	.017	.002	.001
Zn	.000	.013	.002	.003
Br	.000	.006	.000	.001
Pb	.000	.005	.059	.001

Table A5. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.068	.291	.519	.065
EC	.063	.441	.262	.058
NO_3	.065	.257	.739	.187
SO_4	.051	.135	.081	.753
Na	.769	.082	.150	.055
Mg	.183	.686	.114	.071
Al	.052	.832	.066	.061
Si	.056	.927	.099	.067
Cl	1.000	.317	.151	.099
K	.045	.871	.103	.041
Ca	.018	.633	.013	.000
Ti	.054	.884	.106	.045
V	.037	.133	.128	.894
Cr	.057	.832	.119	.072
Mn	.051	.826	.102	.016
Fe	.057	.776	.016	.011
Ni	.040	.181	.131	.989
Cu	.063	.369	.285	.109
Zn	.062	.269	.322	.152
Br	.059	.250	1.000	.125
Pb	.062	.170	.853	.108

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.003	.009	.045	.002
EC	.005	.066	.025	.003
NO_3	.005	.022	.034	.004
SO_4	.003	.011	.011	.060
Na	.117	.019	.015	.001
Mg	.004	.082	.007	.001
Al	.005	.104	.001	.004
Si	.011	.126	.018	.009
Cl	.000	.026	.006	.002
K	.005	.182	.015	.007
Ca	.004	.042	.002	.000
Ti	.011	.106	.012	.008
V	.001	.014	.011	.113
Cr	.016	.113	.027	.013
Mn	.002	.154	.010	.001
Fe	.009	.081	.003	.002
Ni	.007	.004	.008	.018
Cu	.003	.033	.013	.002
Zn	.001	.034	.027	.003
Br	.009	.019	.000	.010
Pb	.004	.005	.072	.009

Table A5. Continued

MEANSPINSBETA	MARINE	UDUST	AUTO	RDOIL
OC	.004	.091	.233	.004
EC	.004	.212	.062	.003
NO_3	.004	.076	.520	.034
SO_4	.003	.027	.008	.708
Na	.593	.008	.022	.003
Mg	.038	.641	.014	.006
Al	.003	.915	.005	.004
Si	.003	.989	.009	.004
Cl	1.000	.120	.022	.010
K	.002	.756	.009	.001
Ca	.000	.569	.000	.000
Ti	.003	.957	.011	.002
V	.002	.026	.019	.963
Cr	.003	.747	.012	.005
Mn	.003	.906	.012	.000
Fe	.003	.725	.000	.000
Ni	.002	.038	.016	.940
Cu	.004	.149	.072	.011
Zn	.004	.084	.098	.023
Br	.004	.076	1.000	.016
Pb	.005	.041	.828	.014

STDSPINSBETA	MARINE	UDUST	AUTO	RDOIL
OC	.000	.011	.007	.000
EC	.000	.014	.006	.000
NO_3	.001	.009	.046	.004
SO_4	.000	.005	.001	.021
Na	.089	.003	.002	.001
Mg	.003	.090	.001	.001
Al	.000	.081	.000	.000
Si	.001	.018	.001	.000
Cl	.000	.015	.001	.001
K	.000	.096	.000	.000
Ca	.000	.078	.000	.000
Ti	.001	.064	.001	.000
V	.000	.004	.002	.064
Cr	.001	.056	.001	.001
Mn	.000	.084	.000	.000
Fe	.000	.033	.000	.000
Ni	.000	.006	.001	.057
Cu	.000	.017	.003	.001
Zn	.000	.013	.002	.004
Br	.001	.004	.000	.001
Pb	.001	.003	.046	.001

Table A5. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.064	.301	.483	.061
EC	.060	.460	.248	.056
NO_3	.064	.276	.721	.185
SO_4	.057	.165	.089	.841
Na	.769	.089	.148	.055
Mg	.196	.799	.120	.076
Al	.055	.956	.069	.064
Si	.055	.995	.095	.066
Cl	1.000	.346	.149	.099
K	.042	.868	.094	.037
Ca	.019	.753	.014	.000
Ti	.054	.978	.106	.046
V	.041	.160	.139	.981
Cr	.054	.864	.111	.069
Mn	.054	.951	.107	.017
Fe	.057	.851	.016	.011
Ni	.039	.194	.127	.969
Cu	.060	.385	.269	.105
Zn	.061	.290	.313	.151
Br	.059	.276	1.000	.126
Pb	.067	.201	.910	.117

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.002	.019	.007	.002
EC	.000	.015	.012	.003
NO_3	.007	.015	.032	.010
SO_4	.003	.015	.007	.013
Na	.057	.016	.008	.005
Mg	.008	.055	.004	.005
Al	.002	.043	.001	.001
Si	.005	.009	.005	.003
Cl	.000	.021	.004	.003
K	.004	.054	.002	.002
Ca	.003	.052	.002	.000
Ti	.006	.033	.004	.004
V	.004	.012	.008	.033
Cr	.007	.033	.005	.004
Mn	.004	.044	.002	.001
Fe	.004	.020	.003	.001
Ni	.006	.015	.004	.029
Cu	.001	.021	.006	.006
Zn	.003	.022	.004	.013
Br	.009	.007	.000	.005
Pb	.005	.008	.025	.006

Table A6. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 5

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.018	.059	.097	.040
EC	.016	.092	.042	.031
NO_3	.084	.229	.570	.123
SO_4	.093	.249	.152	.785
Na	.730	.088	.111	.137
Mg	.139	.431	.062	.074
Al	.039	.359	.046	.029
Si	.039	.413	.048	.023
Cl	.760	.217	.100	.247
K	.013	.238	.031	.042
Ca	.027	.656	.011	.006
Ti	.027	.283	.045	.023
V	.032	.082	.065	.345
Cr	.035	.527	.074	.152
Mn	.025	.245	.046	.010
Fe	.065	.540	.035	.019
Ni	.025	.081	.056	.523
Cu	.060	.265	.167	.193
Zn	.023	.098	.092	.252
Br	.012	.070	.176	.114
Pb	.098	.269	.963	.390

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.008	.020	.036	.051
EC	.006	.037	.002	.043
NO_3	.072	.181	.490	.058
SO_4	.092	.277	.143	.373
Na	.271	.026	.007	.191
Mg	.175	.445	.061	.088
Al	.036	.290	.048	.023
Si	.047	.513	.050	.008
Cl	.415	.196	.067	.369
K	.004	.167	.015	.062
Ca	.017	.220	.004	.004
Ti	.020	.138	.034	.014
V	.040	.101	.072	.140
Cr	.013	.430	.043	.238
Mn	.027	.199	.053	.007
Fe	.070	.403	.038	.013
Ni	.019	.045	.028	.408
Cu	.026	.087	.028	.250
Zn	.012	.107	.072	.404
Br	.010	.069	.166	.186
Pb	.024	.090	.065	.528

Table A6. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.002	.119	.221	.006
EC	.002	.268	.046	.003
NO_3	.002	.128	.410	.038
SO_4	.001	.064	.016	.930
Na	.318	.027	.030	.006
Mg	.012	.703	.015	.006
Al	.001	.975	.007	.005
Si	.001	.940	.010	.004
Cl	1.000	.316	.053	.024
K	.001	.771	.010	.002
Ca	.000	.645	.000	.000
Ti	.001	.953	.012	.002
V	.001	.045	.022	.855
Cr	.001	.704	.013	.003
Mn	.001	.897	.013	.000
Fe	.001	.684	.001	.000
Ni	.001	.066	.021	.926
Cu	.002	.209	.062	.014
Zn	.002	.099	.080	.028
Br	.002	.138	.900	.021
Pb	.002	.089	.866	.020

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.001	.014	.070	.001
EC	.000	.017	.014	.001
NO_3	.000	.004	.087	.010
SO_4	.000	.011	.004	.086
Na	.079	.011	.011	.002
Mg	.003	.087	.003	.001
Al	.000	.040	.002	.000
Si	.000	.060	.003	.000
Cl	.000	.005	.017	.002
K	.000	.070	.002	.000
Ca	.000	.075	.000	.000
Ti	.000	.061	.003	.000
V	.000	.007	.002	.146
Cr	.000	.145	.005	.000
Mn	.000	.023	.003	.000
Fe	.000	.028	.000	.000
Ni	.000	.010	.001	.128
Cu	.000	.037	.018	.003
Zn	.000	.003	.029	.006
Br	.001	.025	.088	.007
Pb	.001	.021	.233	.002

Table A6. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.077	.379	.636	.100
EC	.074	.619	.311	.082
NO_3	.071	.389	.866	.253
SO_4	.039	.192	.117	.872
Na	.892	.165	.219	.093
Mg	.162	.792	.140	.088
Al	.043	.861	.088	.072
Si	.038	.795	.100	.065
Cl	1.000	.363	.184	.122
K	.034	.844	.118	.046
Ca	.022	.912	.016	.006
Ti	.043	.892	.124	.053
V	.036	.183	.159	.958
Cr	.051	.938	.157	.078
Mn	.042	.854	.124	.023
Fe	.055	.949	.052	.022
Ni	.036	.221	.153	.984
Cu	.073	.501	.336	.157
Zn	.077	.367	.410	.233
Br	.050	.294	.931	.137
Pb	.063	.247	.941	.142

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.011	.030	.114	.008
EC	.001	.074	.037	.011
NO_3	.009	.035	.180	.031
SO_4	.010	.047	.016	.115
Na	.015	.022	.031	.008
Mg	.021	.087	.011	.004
Al	.004	.122	.003	.008
Si	.004	.114	.019	.008
Cl	.000	.032	.042	.019
K	.004	.020	.016	.002
Ca	.005	.084	.004	.003
Ti	.005	.123	.008	.006
V	.005	.022	.013	.060
Cr	.001	.055	.017	.004
Mn	.006	.126	.011	.003
Fe	.006	.046	.007	.003
Ni	.002	.033	.002	.027
Cu	.006	.082	.063	.024
Zn	.012	.018	.109	.012
Br	.009	.028	.060	.017
Pb	.016	.033	.052	.020

Table A6. Continued

MEANSPINSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.005	.118	.284	.008
EC	.004	.280	.062	.005
NO_3	.004	.117	.489	.046
SO_4	.002	.049	.016	.948
Na	.557	.019	.028	.006
Mg	.030	.707	.019	.008
Al	.002	.978	.009	.006
Si	.002	.946	.013	.006
Cl	1.000	.129	.028	.013
K	.001	.788	.013	.002
Ca	.000	.668	.000	.000
Ti	.002	.958	.016	.003
V	.001	.035	.023	.898
Cr	.002	.722	.018	.005
Mn	.002	.907	.017	.001
Fe	.002	.708	.002	.000
Ni	.001	.051	.021	.950
Cu	.005	.215	.084	.020
Zn	.005	.102	.108	.038
Br	.003	.107	.928	.022
Pb	.005	.071	.900	.021

STDSPINSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.001	.015	.071	.001
EC	.001	.018	.016	.001
NO_3	.001	.003	.078	.012
SO_4	.000	.007	.003	.062
Na	.075	.008	.008	.002
Mg	.005	.076	.004	.001
Al	.001	.036	.002	.000
Si	.000	.054	.003	.000
Cl	.000	.012	.009	.002
K	.000	.065	.002	.000
Ca	.000	.071	.000	.000
Ti	.000	.055	.003	.000
V	.000	.005	.001	.104
Cr	.001	.135	.005	.000
Mn	.000	.020	.003	.000
Fe	.000	.027	.000	.000
Ni	.000	.007	.000	.087
Cu	.001	.036	.020	.004
Zn	.001	.004	.033	.007
Br	.001	.011	.065	.006
Pb	.001	.015	.173	.002

Table A6. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.070	.342	.530	.087
EC	.064	.529	.248	.067
NO_3	.063	.342	.698	.214
SO_4	.045	.220	.126	.973
Na	.745	.137	.167	.074
Mg	.174	.840	.139	.090
Al	.050	.989	.095	.079
Si	.047	.972	.114	.076
Cl	1.000	.358	.167	.115
K	.036	.887	.115	.047
Ca	.019	.817	.014	.005
Ti	.047	.978	.127	.056
V	.038	.188	.151	.946
Cr	.047	.847	.132	.068
Mn	.048	.952	.129	.025
Fe	.050	.841	.042	.018
Ni	.038	.226	.146	.974
Cu	.069	.463	.288	.140
Zn	.067	.320	.326	.195
Br	.056	.327	.963	.147
Pb	.067	.266	.945	.146

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.008	.022	.065	.005
EC	.004	.017	.032	.008
NO_3	.006	.005	.056	.028
SO_4	.001	.015	.011	.032
Na	.051	.027	.023	.011
Mg	.014	.045	.013	.006
Al	.005	.018	.009	.003
Si	.005	.028	.013	.002
Cl	.000	.017	.028	.008
K	.004	.036	.008	.003
Ca	.003	.043	.004	.002
Ti	.004	.028	.011	.004
V	.006	.013	.003	.056
Cr	.007	.079	.020	.002
Mn	.005	.011	.011	.001
Fe	.004	.016	.001	.000
Ni	.005	.015	.002	.045
Cu	.006	.038	.035	.015
Zn	.005	.007	.048	.019
Br	.010	.017	.033	.019
Pb	.007	.028	.094	.007

Table A7. Mean and standard deviation of three simulation runs for MPIN and other diagnostics for data set 6

MEANSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.013	.050	.094	.018
EC	.045	.282	.196	.029
NO_3	.062	.443	.616	.262
SO_4	.015	.090	.042	.370
Na	.708	.094	.137	.080
Mg	.123	.603	.100	.070
Al	.012	.234	.021	.020
Si	.026	.410	.072	.034
Cl	1.000	.385	.194	.129
K	.008	.231	.043	.013
Ca	.012	.383	.004	.003
Ti	.022	.372	.051	.022
V	.021	.066	.076	.468
Cr	.050	.737	.135	.063
Mn	.050	.760	.134	.021
Fe	.030	.497	.023	.010
Ni	.040	.210	.142	1.000
Cu	.061	.356	.264	.115
Zn	.029	.135	.130	.105
Br	.053	.357	.902	.180
Pb	.042	.165	.612	.090

STDSDFBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.002	.015	.028	.005
EC	.052	.311	.246	.027
NO_3	.049	.492	.399	.319
SO_4	.003	.092	.025	.247
Na	.286	.022	.035	.071
Mg	.056	.352	.066	.042
Al	.007	.184	.012	.016
Si	.035	.512	.107	.042
Cl	.000	.104	.057	.028
K	.010	.270	.061	.016
Ca	.012	.326	.004	.003
Ti	.017	.223	.039	.013
V	.015	.018	.053	.301
Cr	.017	.130	.075	.010
Mn	.031	.345	.093	.011
Fe	.022	.463	.018	.008
Ni	.009	.081	.022	.000
Cu	.050	.265	.269	.087
Zn	.027	.141	.107	.129
Br	.012	.165	.097	.111
Pb	.027	.084	.434	.038

Table A7. Continued

MEANSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.003	.100	.310	.007
EC	.003	.309	.078	.003
NO_3	.002	.182	.629	.034
SO_4	.001	.053	.017	.705
Na	.501	.031	.045	.007
Mg	.015	.752	.020	.006
Al	.001	.919	.009	.004
Si	.001	.998	.014	.004
Cl	1.000	.340	.077	.021
K	.001	.818	.013	.001
Ca	.000	.734	.000	.000
Ti	.001	.930	.016	.002
V	.001	.046	.032	.818
Cr	.001	.826	.020	.004
Mn	.001	.893	.017	.000
Fe	.002	.809	.002	.000
Ni	.001	.076	.034	1.000
Cu	.002	.173	.079	.011
Zn	.002	.091	.116	.023
Br	.002	.147	.948	.019
Pb	.002	.090	.824	.019

STDSDFSBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.000	.015	.014	.004
EC	.000	.048	.013	.003
NO_3	.000	.012	.095	.028
SO_4	.001	.020	.009	.059
Na	.051	.024	.009	.007
Mg	.004	.067	.003	.003
Al	.000	.033	.002	.002
Si	.000	.003	.003	.002
Cl	.000	.037	.011	.003
K	.000	.103	.002	.000
Ca	.000	.034	.000	.000
Ti	.000	.052	.002	.001
V	.000	.030	.013	.107
Cr	.000	.139	.002	.004
Mn	.000	.139	.004	.000
Fe	.000	.029	.001	.000
Ni	.000	.025	.011	.000
Cu	.000	.018	.011	.010
Zn	.001	.032	.037	.014
Br	.001	.037	.090	.009
Pb	.000	.004	.154	.015

Table A7. Continued

MEANSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.076	.333	.679	.119
EC	.075	.581	.337	.076
NO_3	.061	.380	.827	.200
SO_4	.042	.200	.130	.971
Na	1.000	.164	.248	.106
Mg	.158	.811	.155	.090
Al	.044	.811	.090	.069
Si	.038	.724	.097	.061
Cl	.860	.359	.199	.119
K	.030	.882	.132	.048
Ca	.023	.777	.013	.008
Ti	.045	.864	.131	.051
V	.038	.172	.170	.995
Cr	.053	.890	.161	.080
Mn	.046	.851	.132	.022
Fe	.048	.757	.044	.017
Ni	.029	.165	.127	.793
Cu	.091	.568	.444	.181
Zn	.086	.373	.491	.246
Br	.037	.267	.798	.134
Pb	.056	.271	.944	.154

STDSPINBETA

	MARINE	UDUST	AUTO	RDOIL
OC	.002	.054	.023	.030
EC	.008	.078	.030	.046
NO_3	.013	.052	.195	.048
SO_4	.010	.057	.037	.027
Na	.000	.066	.022	.051
Mg	.014	.120	.042	.007
Al	.003	.087	.008	.019
Si	.009	.186	.016	.025
Cl	.023	.006	.017	.005
K	.007	.028	.018	.004
Ca	.003	.099	.007	.005
Ti	.005	.090	.024	.009
V	.006	.057	.020	.009
Cr	.011	.191	.034	.042
Mn	.013	.241	.032	.006
Fe	.004	.049	.008	.003
Ni	.004	.048	.027	.041
Cu	.009	.065	.051	.073
Zn	.012	.065	.091	.073
Br	.004	.055	.179	.067
Pb	.007	.027	.059	.032

Table A7. Continued

MEANSPINSBETA	MARINE	UDUST	AUTO	RDOIL
OC	.006	.096	.373	.010
EC	.006	.315	.098	.004
NO_3	.004	.158	.678	.039
SO_4	.002	.043	.018	.782
Na	.707	.020	.036	.006
Mg	.033	.751	.024	.008
Al	.003	.927	.011	.005
Si	.003	.999	.017	.005
Cl	1.000	.158	.045	.014
K	.001	.831	.017	.002
Ca	.001	.751	.000	.000
Ti	.003	.937	.020	.003
V	.002	.036	.031	.873
Cr	.003	.835	.025	.006
Mn	.003	.902	.021	.000
Fe	.004	.823	.003	.000
Ni	.002	.056	.031	1.000
Cu	.005	.179	.101	.016
Zn	.005	.093	.147	.032
Br	.003	.120	.961	.021
Pb	.004	.077	.864	.021

STDSPINSBETA	MARINE	UDUST	AUTO	RDOIL
OC	.001	.014	.015	.005
EC	.001	.047	.014	.004
NO_3	.001	.008	.089	.030
SO_4	.001	.017	.010	.045
Na	.040	.015	.006	.006
Mg	.009	.059	.004	.003
Al	.000	.030	.003	.002
Si	.000	.002	.004	.003
Cl	.000	.017	.007	.002
K	.001	.094	.002	.001
Ca	.000	.031	.000	.000
Ti	.000	.047	.002	.001
V	.000	.023	.012	.075
Cr	.001	.126	.002	.005
Mn	.000	.128	.005	.000
Fe	.000	.028	.001	.000
Ni	.001	.020	.011	.000
Cu	.001	.018	.014	.013
Zn	.001	.032	.044	.018
Br	.001	.028	.067	.010
Pb	.000	.007	.120	.014

Table A7. Continued

MEANNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.075	.310	.611	.097
EC	.077	.560	.313	.062
NO_3	.066	.397	.822	.190
SO_4	.046	.204	.130	.884
Na	.840	.133	.190	.074
Mg	.179	.866	.156	.087
Al	.055	.963	.103	.071
Si	.055	.999	.131	.072
Cl	1.000	.397	.211	.116
K	.033	.911	.130	.044
Ca	.027	.867	.013	.008
Ti	.053	.968	.140	.050
V	.042	.183	.175	.934
Cr	.057	.912	.158	.072
Mn	.054	.948	.144	.021
Fe	.060	.907	.050	.018
Ni	.044	.233	.175	1.000
Cu	.071	.423	.318	.120
Zn	.073	.301	.380	.174
Br	.051	.344	.980	.144
Pb	.060	.276	.928	.141

STDNMPIN

	MARINE	UDUST	AUTO	RDOIL
OC	.004	.022	.012	.022
EC	.005	.042	.023	.029
NO_3	.005	.010	.054	.073
SO_4	.013	.041	.036	.025
Na	.024	.060	.016	.036
Mg	.024	.034	.012	.019
Al	.001	.016	.014	.016
Si	.000	.001	.014	.017
Cl	.000	.022	.016	.007
K	.008	.051	.009	.007
Ca	.004	.018	.006	.005
Ti	.002	.024	.008	.011
V	.005	.059	.033	.039
Cr	.005	.068	.007	.032
Mn	.004	.069	.016	.002
Fe	.000	.015	.009	.002
Ni	.006	.043	.031	.000
Cu	.004	.021	.022	.049
Zn	.009	.054	.061	.048
Br	.010	.042	.034	.031
Pb	.003	.012	.063	.046

Table A8. Effects of deletion of influential and nonifluential elements to source apportionments and their variance for data set 6

	Source apportionment				Standard error of source apportionment			
Deleted elements	Marine	Udust	Auto	Rdoil	Marine	Udust	Auto	Rdoil
None	2.10	36.62	11.00	4.85	.41	2.76	1.31	.65
Na	1.68	36.41	11.22	4.81	.53	2.77	1.32	.65
Cl	2.61	35.99	11.25	4.78	.63	2.83	1.33	.66
Na,Cl	.92	36.83	11.16	4.84	2.29	3.03	1.34	.66
Si,Ti,Cr,Mn	2.15	34.16	11.27	4.93	.41	3.56	1.34	.65
Zn	2.10	36.63	11.01	4.85	.41	2.78	1.34	.66
EC,Cu,Zn	2.09	36.80	11.07	4.85	.41	2.88	1.40	.66
OC,EC,Cu,Zn	2.08	36.94	11.25	4.85	.41	2.92	1.52	.66
Cl,Mn,Ni,Br	2.73	32.67	12.86	5.29	.63	3.01	1.62	.84

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA 450/4-88-005		

4. TITLE AND SUBTITLE	5. REPORT DATE
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Dr. Ronald C. Henry and Mr. Bong Mann Kim	

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16. ABSTRACT

This document (1) describes diagnostics which will assist the CMB user in identifying the most influential species in CMB calculations; (2) demonstrates testing done on diagnostics by using sets of artificial data and intercomparisons among diagnostics; and (3) recommends a modification of the pseudo-inverse matrix (MPIN) diagnostic to be used in identifying influential species. Influential species are those which have large effect on the estimated source contributions or its error.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Diagnostics Chemical Mass Balance Influential species MPIN Diagnostic		

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