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BRAVO & Using Factor Analysis to Relate Aerosol Concentrations
to Light Extinction**

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Abstract

The U.S. EPA's Regional Haze Rule stipulates use of the reconstruction equation for calculating light extinction (b_{ext}) in Class I areas. Because the Big Bend Regional Aerosol and Visibility Observational (BRAVO) Study collected daily data during July through October in 1999, the Study presented an opportunity to compare measured b_{ext} (from a transmissometer) to reconstructed b_{ext} for that period. While reconstructed b_{ext} correlated well with daily mean b_{ext} at the BIBE1 (Big Bend 1) transmissometer in both seasons during the study period ($R^2 \sim 0.9$), measured values were typically higher at this site. This analysis also examined data from another transmissometer operating during the Study, BBEP (East Path). Correlations between measured and reconstructed b_{ext} at this instrument were comparable to BIBE1, but the tendency of the equation to under- or over-predict b_{ext} depended on whether additional lamp brightening adjustments were made to the hourly data. R^2 values ranged 0.85 to 0.89.

Regression fits of measured b_{ext} to the reconstruction equation variables did not estimate coefficients that were consistent with the literature in either season. However, there was evidence of multicollinearity between variables, which compromises the ability of a regression model to accurately estimate coefficients (but not the predictive capacity of the model itself). Results showed a strong correlation with equation components but could only identify some components of the reconstruction equation as significant predictors of b_{ext} .

To address the collinearity problem and reconstruct b_{ext} a different way, the TCEQ explored factor analysis as a method to relate aerosol data to b_{ext} . The method identified five underlying factors, with the two strongest factors related to soil materials and sulfates. Regression analysis using factor scores and b_{ext} data achieved R^2 values ranging from 0.74 to 0.89 and provided some information about sources affecting visibility at the park. Factors indicating influence from coal burning and smelting, as well as from soil and nitrate sources could be related to b_{ext} . However, findings are limited to the BRAVO data set; this technique did not generate a "new" reconstruction equation for Big Bend.

Introduction

The reconstruction equation (Malm et al., 1996) relates concentrations of sulfates, nitrates, organic carbon mass (OMC), light absorbing carbon (LAC), fine soil, and coarse mass (CM) to light extinction (b_{ext}). This equation must be used for calculating b_{ext} in Class I areas under EPA's Regional Haze Rule (40 CFR 51, 1999). The **Reconstruction Equation (Equation 1)** is defined as:

$$b_{\text{ext}} = (3)f(\text{RH})[\text{Sulfate}] + (3)f(\text{RH})[\text{Nitrate}] + (4)[\text{OMC}] + (10)[\text{LAC}] + (1)[\text{Fine Soil}] + (0.6)[\text{CM}] + 10$$

where [species] is the average concentration in $\mu\text{g}/\text{m}^3$, and b_{ext} is in inverse Megameters (Mm^{-1}).

As b_{ext} increases, visibility decreases. Because the growth of aerosols from water uptake (hygroscopicity) is dependent upon relative humidity (RH), an adjustment factor called $f(\text{RH})$ must be included in the equation. This factor adjusts the light scattering effect of hygroscopic aerosol species as humidity increases (Malm et al., 1996). The Rayleigh constant, or the light scattering attributed to gas molecules in the atmosphere, is assumed to be 10 Mm^{-1} (EPA, 2001b). Sulfates and nitrates are assumed to be present as ammonium sulfate and ammonium nitrate (EPA, 2001b).

Analysis and Results

This analysis used the BRAVO aerosol data set created April 5, 2002 by the University of California at Davis. Hourly b_{ext} and relative humidity data came from the BRAVO BIBE1 transmissometer data set as of April 6, 2001, generated by Air Resource Specialists, Inc. (ARS) and compiled by Desert Research Institute (DRI). Statistical significance tests relied upon a 0.05 significance level.

This analysis used 24-hour average particulate matter (PM) species concentration data collected at Big Bend during BRAVO to reconstruct daily average b_{ext} . Instead of EPA's site-specific monthly average $f(\text{RH})$ values (EPA, 2001b, App. A), daily average $f(\text{RH})$ was calculated from hourly RH data converted into $f(\text{RH})$ values (EPA, 2001a, Table 4-2). To assure the most appropriate comparison to transmissometer data, only hours with both acceptable b_{ext} and RH data were included in the average.

Aerosol data was collected at Big Bend's IMPROVE (Interagency Monitoring of Protected Visual Environments) network sampler (BIBED, BIBE3) and K-bar locations (C024T, C024) during the Study. It should be noted that the sampling configuration initially included the IMPROVE site and shifted to the K-bar sites on July 23 (C024) and August 10 (C024T). Data filtering omitted invalid aerosol data and replaced most species below the minimum detection level (MDL) with zero. Data with high flow and low flow flags were included in this analysis. Because organic and elemental carbon components are summed to yield OMC and LAC estimates, all valid concentrations of these species were used as reported. Before reconstructing b_{ext} , any negative values for OMC, LAC, or CM were replaced with zero. Aerosol data on July 6 through July 8 were omitted because some samplers were not operating properly and only provided field blanks.

The BIBE1 transmissometer (part of the IMPROVE network) at Big Bend National Park is located at 29.30° latitude and -103.18° longitude (approximately 5 kilometers NNW of the K-bar site), 1052 meters elevation. Hourly transmissometer measurements associated with RH below 90 percent were used to calculate daily average b_{ext} . The 90 percent cutoff was intended to prevent possible fog or precipitation from being considered haze events. To correspond with BRAVO aerosol samples, a day was defined as 8:00 AM to 8:00 AM the following day. Daily averages were kept if at least 15 hours were valid. To capture any rapidly building haze events, this analysis did include hours with the interference flag indicating the change in b_{ext} during the hour was above the maximum threshold, as long as b_{ext} was below the maximum 632 Mm^{-1} and RH was below 90 percent.

Linear regression was then used to fit daily average measured b_{ext} to reconstructed b_{ext} . Ideally, the intercept of the regression line should be zero, and the slope equal to one. With a slope of 1.2, measured b_{ext} tended to be higher on average than reconstructed b_{ext} , especially at higher values. The adjusted correlation coefficient (R^2) was 0.89, or reconstructed b_{ext} explained 89

percent of the variance in measured b_{ext} (**Figure 1**).

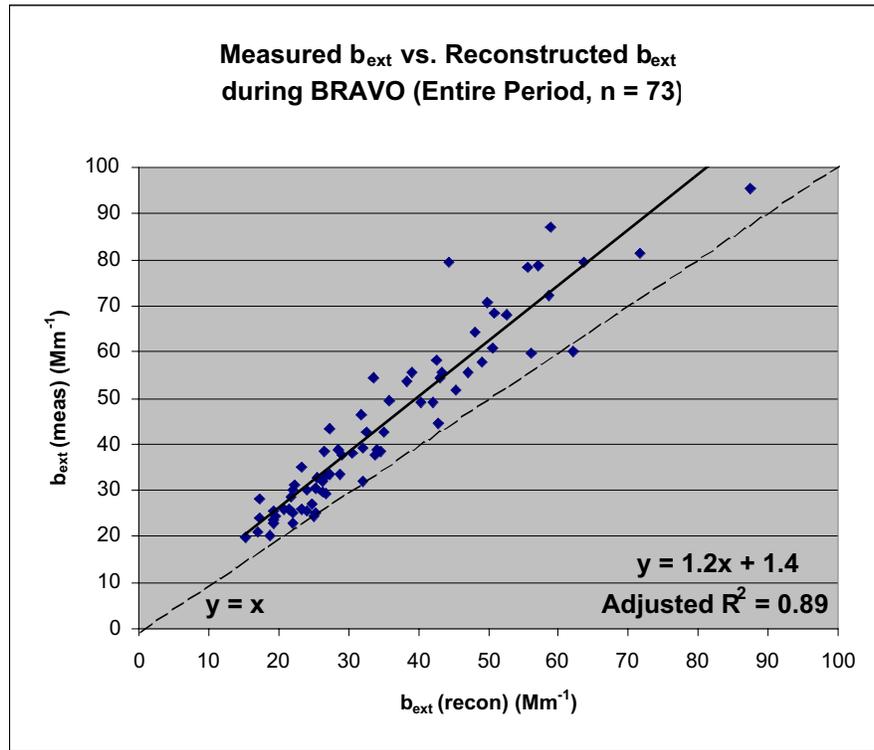


Figure 1–BRAVO Period b_{ext} Comparison at BIBE1

The coefficient b_{ext} can be converted into deciview (dv), which must be used to track progress under the Regional Haze Rule (EPA, 2001b). The deciview is a logarithmically-scaled haze index and is defined by **Equation 2**:

$$dv = 10 * \ln(b_{ext}/10)$$

One deciview is approximately equal to the change necessary to *perceive* a change in visibility. As with b_{ext} , visibility worsens as the deciview value increases. Because the logarithmic transformation changes the distribution, the correlation between measured and reconstructed deciview values looks somewhat different (**Figure 2**). The R^2 was 0.91, and the slope was 1.0. The intercept, however, was statistically greater than zero at 1.9.

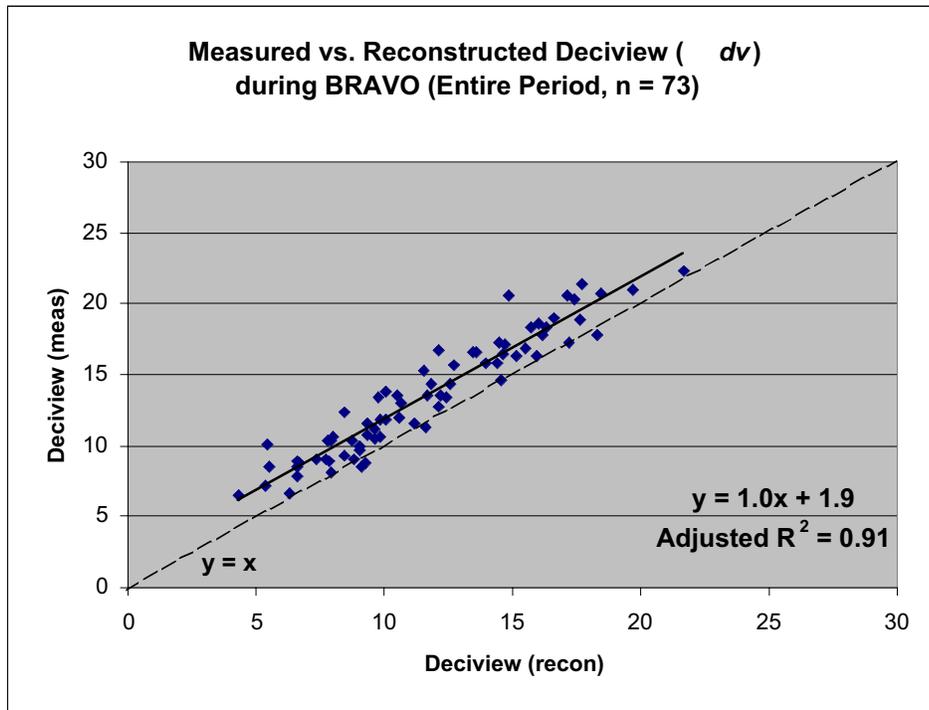


Figure 2 – BRAVO Period dv Comparison at BIBE1

Grouped by season, results were similar to one another. A total of 52 days had sufficient data to be compared in the fall (September through October), while only 21 days had enough usable data in the summer (July through August). A major limitation was the lack of PM_{10} data (used to calculate CM) in the first two months of the Study. For b_{ext} , the R^2 was 0.90 in the fall and 0.85 in the summer (**Figures 3 and 4**). The dashed line is the reference line, $y = x$. The slope in both cases suggests the difference between measured and reconstructed b_{ext} grows as the values increase. However, translated into deciview, the slopes are closer to one, with intercepts statistically greater than zero.

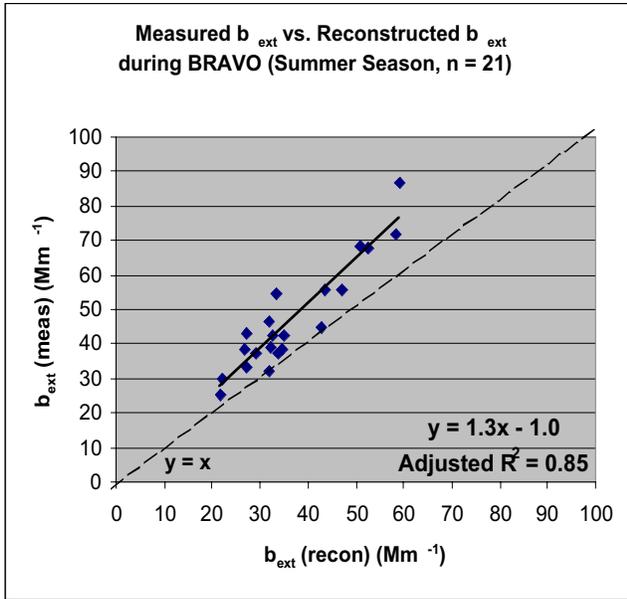


Figure 3 – Summer (BIBE1)

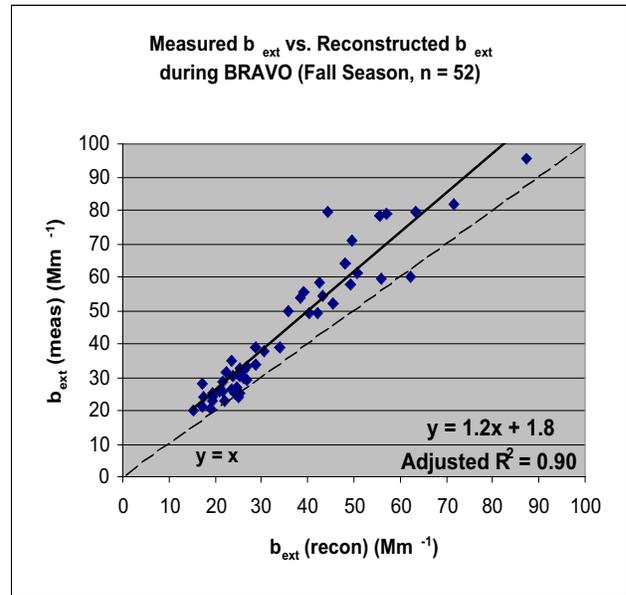


Figure 4 – Fall (BIBE1)

It was possible that summer discrepancies could be attributed to sampling location changes. Therefore, it was useful to check the summertime fit during the period after August 10. This restriction modestly improved results ($R^2 = 0.91$, intercept = 0.93, and slope = 1.3), but also left about half the number of data points (11).

A Wilcoxon Matched-Pairs Signed-Ranks Test (non-parametric significance test) was used to assess if differences between measured and reconstructed daily light extinction values were significant. Because predicted slopes in the deciview correlations were close to one, the test was applied to dv values. Results confirmed reconstructed and measured deciview values in both the summer and fall were significantly different at the 0.05 level.

Multiple linear regression was then used to fit measured b_{ext} to the components of the reconstruction equation: $f(RH) \cdot \text{sulfate}$, $f(RH) \cdot \text{nitrate}$, OMC, LAC, fine soil, and CM. **Table 1** shows coefficients predicted by both regression models, the number of points (N), and standard deviation of the error; standard error is noted in parentheses. Most of the coefficients were not consistent with the reconstruction equation, but some were closer than others. This outcome may be the result of collinearity influences, which will be discussed later.

Table 1 – Regression Model Coefficients for Reconstructed Light Extinction (BRAVO)

Season	N	Std. Dev. of Error	Intercept (Mm^{-1})	$f(RH) \times \text{Sulfate}$	$f(RH) \times \text{Nitrate}$	OMC	Fine Soil	LAC	CM	Adj. R^2
<i>Summer</i>	21	4.0	18.0 (2.6)	5.9 (0.5)	-9.9 (4.0)	2.6 (1.4)	3.2 (1.0)	3.9 (10.9)	-0.49 (0.45)	0.94
<i>Fall</i>	52	6.3	14.3 (1.9)	4.1 (0.3)	3.6 (4.9)	5.2 (2.1)	2.2 (3.9)	-11.7 (16.2)	0.58 (0.42)	0.90
<i>Reconstruction Equation [Malm, 1996]</i>	-	-	10	3	3	4	1	10	0.6	-

During the fall months of BRAVO, the sulfate and OMC terms, and the intercept (what should be the Rayleigh scattering constant) were significant at the 0.05 level. If the insignificant terms were removed from the regression model, the correlation coefficient in the fall was 0.88. However, when *either* the CM or fine soil terms were included, the R^2 was 0.90, and all three terms were significant. This result was an early indication of possible collinearity problems. In the summer model, the sulfate, nitrate, and fine soil terms, and the intercept were significant at the 0.05 level. When the insignificant terms were removed from the model, the nitrate term also became insignificant, leaving only the sulfate and fine soil terms. Using just these two terms dropped the correlation coefficient considerably to 0.65.

At this point it becomes necessary to address the problem of multicollinearity, suspected among variables in both seasons. Development of the reconstruction equation was not a process simply involving one multiple regression fit to principal aerosol concentrations (Malm et al., 1996), and it is not surprising that variables like fine soil and CM could be collinear. Tolerance valuesⁱ below 0.25 in the summer model indicated collinearity might be a problem with the fine soil term, and the fall model signaled possible interference from the fine soil, OMC, and LAC variables. Collinearity poses a significant difficulty in estimating parameters in any linear regression model, though it does not compromise the predictive capacity of the model itself or prevent determination of which variables have predictive capability in the presence of the other variables (Dallal, 2002; Berry & Feldman, 1985). Regardless, this complication prompted an alternative approach to relating BRAVO PM concentrations to optical b_{ext} data.

Exploratory Factor Analysis

One way to hurdle the multicollinearity obstacle was to use factor analysis. Factor analysis is a method of reducing several variables (species concentrations, in this case) into a smaller set of “underlying factors” responsible for covariation in the data (Hatcher, 1994). The term “exploratory” means the number or nature of factors is not already known. The technique assumes the variables are the linear combination of these underlying factors. If these factors are structured orthogonally to one another (i.e., uncorrelated), they might be used to predict a response (such as b_{ext}) without the complication of collinearity.

Unfortunately, the BRAVO PM data set did not fulfill all the assumptions of factor analysis perfectly. Not surprisingly, observed concentrations did not fit a normal distribution (much of air quality data does not). This method also assumes the relationships among all variables are linear, which was not explored. Despite shortcomings of the data, factor analysis was still valuable to understanding what sources could be linked to visibility during the Study.

Factor analysis (using the varimax rotation method) was performed on the subset of BRAVO $\text{PM}_{2.5}$ data from Big Bend 24-hour and 12-hour sample sites. The data set included 37 elements, carbons, and ions. Including 12-hour sites allowed most species to have at least five times as many observations as the number of variables—a recommended minimum for factor analysis (Hatcher, 1994). All species contained at least 75 valid observations, and 27 of the species

ⁱ **Tolerance value** is the fraction of the total variance in one variable that is *not predicted* by the other variables (the $1-R^2$ value of a variable regressed on all the other variables in the model). The inverse of the tolerance value ($1/(1-R^2)$) is called the Variance Inflation Factor (VIF) (Motulsky et al., 1990-1998).

contained 190 or more valid observations. To prevent losing some of the more interesting elements, the TCEQ chose not to omit any species from this set and proceeded with filtering. Filtering screened out invalid concentrations (those reported as '-99') but kept negative concentrations as reported. Twelve days were omitted through this process because so few or no variables had data (July 9 - 11; July 23 - 25; July 29; July 30 - August 1; and October 26 - 28). After filtering, missing data were converted to zero to fill in the data matrix for factor analysis. The final data set contained 270 records with all 37 variables (species). (A later analysis verified that when species with less than 190 observations (PNa, PCr, PMn, Ni, Cu, As, Rb, Sr, NO₂, and Mg²⁺) were omitted, factor structure was very similar.)

This procedure identified five factors. Factor loadings greater than 0.35 were considered significant. **Table 2** summarizes the results and significant factor loading species; see **Appendices A1. and A2.** for complete factor analysis results.

Table 2 – Summary of Factor Analysis Results (Varimax Rotation) for Big Bend Sites, PM_{2.5} Data

	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5
<i>Species</i>	Al, Si, K, Ca, Ti, V, Mn, Fe, Rb, Sr, NO ₃ ⁻ , Na ⁺ , Mg ⁺² , Ca ⁺² , O1	S, H, SO ₄ , NH ₄ ⁺ , Se, Br, O2, O4, OP, E1	Zn, Pb, Br, K ⁺ , Ca ⁺² , O3, O4, E1	O2, O3, OP, E1, E2, E3	Na, Na ⁺ , NO ₃ ⁻ , V (negative loading)
<i>% Variance Explained</i>	33 %	23 %	11 %	10 %	7 %

The first factor (F₁) was most likely associated with soil, with the most prominent factor loadings (>0.90) coming from aluminum (Al), silicon (Si), potassium (K), calcium (Ca), titanium (Ti), and iron (Fe). Other variables with significant loadings on this factor included vanadium (V), nitrate (NO₃⁻), the sodium ion (Na⁺), and one of the organic carbon groups, O1. F₁ accounted for 33 percent of the total variance in the Big Bend aerosol data set. Factor two (F₂), explaining 23 percent of the variance, was sulfate-related, with the heaviest loadings (>0.90) coming from sulfur (S), hydrogen (H), sulfate (SO₄), and ammonium (NH₄⁺). Other important variables loading on this factor were selenium (Se), bromine (Br), organic carbon groups O2 and O4, and elemental carbon group E1. Selenium suggests this second factor is probably associated with coal combustion, a primary source of sulfates (Chow et al., 2002). Factor three (F₃) saw the largest factor loadings (>0.60) from zinc (Zn), lead (Pb), and Br. The K⁺ and Ca⁺² ions, as well as O3, O4, and E1 were also significant. Zinc and lead often indicate smelter influence (Gebhart & Malm, 1997). F₃ explained 11 percent of the variance. Organic and elemental carbon groups O2, O3, OP, E1, E2, and E3 had significant loadings on factor four (F₄), while factor five (F₅) was associated with Na, Na⁺, and NO₃⁻. These factors accounted for 10 and 7 percent of the variance, respectively. The last factor is consistent with other BRAVO findings that suggest nitrates are present as sodium nitrate, rather than ammonium nitrate (W. Malm, personal communication, November 18, 2002; Hand et al., 2001). Interestingly, V had a strong negative loading on F₅ (-0.44), which meant significant vanadium concentrations were not present with the other species that loaded on this factor.

Factor scores were estimated for each record. The next step was to fit these scores to b_{ext} values

in a regression analysis (**Equation 3**). (Essentially, instead of using *species concentrations* to predict daily average b_{ext} during BRAVO, this step used the *underlying factors* that explained the variance in those concentrations during that period.) Because coarse mass (CM) is a major contributor to visibility impairment at Big Bend (CENRAP, July 2002) and because PM_{10} was not included in the factor analysis above, CM had to be brought back into the analysis. While the varimax rotation method ensured the five factors were orthogonal, the question was: would the CM term reintroduce collinearity into the regression fit? A fit of F_1 (soil-related) scores to CM resulted in an R^2 of 0.64 in the fall months, while there was no significant correlation in the summer months. In the summer, however, CM had a significant relationship with sulfate-related F_2 ($R^2 = 0.56$) that was not observed in the fall. Despite potential problems, CM was too important to visibility to be omitted. The goal was to find an equation like **Equation 3**, where constants ‘a’ though ‘f’ represent regression coefficients for the factor score ($F_{n,i}$) and CM concentration terms, fit to daily average b_{ext} (using ‘i’ number of days):

$$b_{\text{ext},i} = a(F_{1,i}) + b(F_{2,i}) + c(F_{3,i}) + d(F_{4,i}) + e(F_{5,i}) + f[\text{CM}]_i$$

Because b_{ext} was a 24-hour average, the regression only included factor scores coupled with 24-hour PM observations—this meant only one record per day (113 days total). Nitrate or sulfate loaded significantly on F_1 , F_2 , and F_5 , and so additional variables were created by multiplying each of these factors by daily average $f(\text{RH})$ to account for hygroscopic behavior ($f\text{RH} * F_1$, $f\text{RH} * F_2$, $f\text{RH} * F_5$). (The assumption was that the relationship with $f(\text{RH})$ was best described as multiplicative.) **Table 3** shows the optimal fits for summer and fall, along with the R^2 values and standard deviation of the error. The optimal fit was the equation with the largest number of significant variables and as many positive coefficients as possible, and was determined by using both backward elimination and stepwise selection techniques.

Table 3 – Multiple Regression Fits of Factor Scores and CM to BIBE1 Daily Average b_{ext}

Season	No. of Days	Adj. R^2	Std. Dev. of Error	Resulting Equation
<i>Summer</i>	23	0.87	5.5	$b_{\text{ext}} = 55.3 + 2.7(f\text{RH} * F_1) + 17.3(F_2) - 1.5(\text{CM})$
<i>Fall</i>	52	0.89	6.8	$b_{\text{ext}} = 37.2 + 12.2(f\text{RH} * F_2) + 3.5(F_3) + 2.2(F_4) + 6.9(F_5) + 0.74(\text{CM})$

Only F_1 (soil-related), F_2 (sulfate-related), and CM were the significant variables in predicting b_{ext} in the summer. In addition to CM, all factors except F_1 were significant in the fall equation. Higher tolerance values (>0.35) suggested that any collinearity between CM and the other variables was not problematic in either model above, though the presence of CM may have been the reason F_1 was not necessary in the fall equation.

CM has a negative coefficient in the summer equation, as in the original regression analysis with the reconstruction equation (**Table 1**). The reason is not entirely clear, but one observation could offer at least part of an explanation. During BRAVO, *higher* CM concentrations in the summer were not only associated with higher sulfate concentrations (and thus larger F_2 scores), but also with *lower* daily mean RH values ($\text{CM} = -0.16 * \text{RH} + 11.6$, $R^2 = 0.33$). It is possible that for these data, subtracting the CM term from the F_2 term somehow models the decreased growth of sulfates under lower RH conditions better than multiplying F_2 by $f(\text{RH})$. It is also possible that CM and/or other species data were flawed for this period. If CM is omitted in the summer, the model explains only about 70 percent of the variance in b_{ext} . Normalizing the CM concentration

data (to correspond to the factors, which were also normalized) did not reverse the sign of the coefficient in the summer, and neither did using F_1 instead of $f(\text{RH}) * F_1$.

In both seasons, the sulfate-related term (F_2) was significant and had the largest coefficient of any variable. This result is consistent with the fact that on average, sulfates are the primary contributor to visibility impairment at Big Bend (**Figures 5 and 6**). Beginning in mid-August, six major sulfate episodes that lasted several days at a time occurred throughout the Study (Ashbaugh et al., 2001). Also, the soil-related factor F_1 was significant in the summer model but not necessary in the fall model. Episodes with elevated fine soil levels were documented in July and early August, and Fe/Ca ratios suggest these periods were associated with Saharan dust transport into the park (Ashbaugh et al., 2001). In **Figure 6**, the fine soil contribution composed only 1 percent of the total reconstructed b_{ext} in the fall season of BRAVO on average, the smallest fraction of all the components for that period and 5 percent less than in the summer.

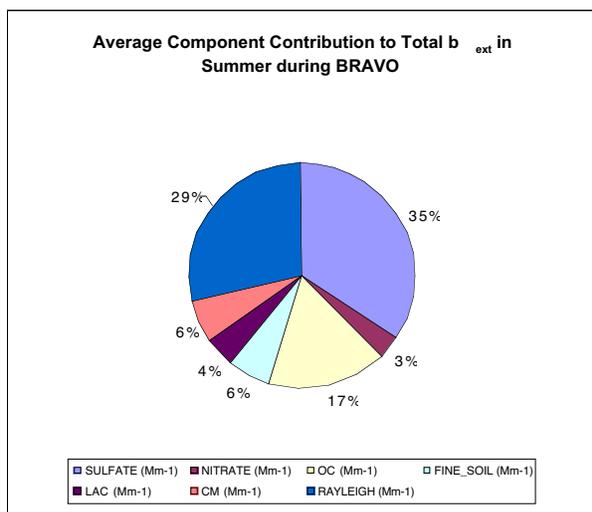


Figure 5 – Average Component Contribution to Total Recon. b_{ext} (Summer)

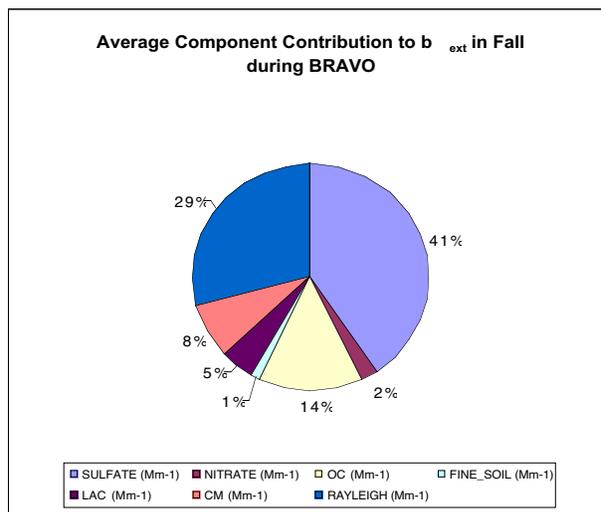


Figure 6 – Average Component Contribution to Total Recon. b_{ext} (Fall)

It is interesting that F_5 was a significant predictor in the fall but not in the summer (**Table 3**); vanadium's (V) strong *negative* loading on F_5 indicated the element's *absence* was associated with this factor. This observation parallels the reduced probability of air mass transport in the fall months through central and northeastern Mexico (Schichtel & Gebhart, 2001), a region associated with high V concentrations (Gebhart et al., 2000). Vanadium had a significant positive loading on F_1 , which was important in the summer—a time when air mass transport from Mexico is more common and when V concentrations were higher during BRAVO (Gebhart et al., 2001). The loading of nitrate on both these factors suggests a seasonal difference in nitrate sources, with one associated with transport from Mexico.

Other conclusions are difficult to draw, but ideas raise possibilities worth further investigation. For example, the absence of F_4 in the summer model could indicate a shift in organic and/or elemental carbon sources between the seasons. Characterization of organic aerosols during BRAVO suggests primary biogenic emissions were small contributors to PM-fine organic matter during the first three months of BRAVO, but shifting wind patterns introduced stronger biogenic influences in October (Brown et al., 2002). Also, smelting influences appear to play some role in visibility at the park.

It is important to remember that while some factors appeared to coincide with one source (or even a combination of sources), most of these factors were constructed from more than one type of species affecting visibility. For example, even though F_4 was not significant in the summer model, the conclusion is not that organic and elemental carbon species were not important to visibility those months; both F_1 and F_2 contained influences from organics and elemental carbon.

While this approach reduces collinearity problems in relating b_{ext} to PM concentrations, it does not yield a “new” reconstruction equation for Big Bend. Instead, factor analysis was a different way to examine what sources contributed to b_{ext} during the BRAVO period. At BIBE1, the outcome was comparable to using the reconstruction equation, with R^2 values close to 0.9 and standard deviation of errors between 4.0 and 7.0.

Comparing Other BRAVO Transmissometers

Originally this analysis also included historical optical data from the IMPROVE transmissometer BIBE1. However, even though BRAVO data from this instrument were acceptable, unresolved problems prompted removal of historical data from the IMPROVE website as of November 2002. Two additional transmissometers operated during the BRAVO Study: BBEP (East Path) and BBWP (West Path). These instruments operated back-to-back, approximately along the same path and about 0.5 km SW of the K-bar site. Prior to August 19, the BBWP transmissometer experienced problems with its feedback block, which prevented post-calibration and rendered the optical data collected until then unusable (J. Molenaar (ARS), personal communication, August 9, 2001). Therefore, the TCEQ compared reconstructed b_{ext} to BBEP measurements.

The initial comparison at BBEP used the same methods described earlier for BIBE1 transmissometer data. **Figure 7** shows reconstructed and measured b_{ext} correlate similarly well for BBEP, with an R^2 value of 0.87, an intercept around 2.3 Mm^{-1} , and a slope of 1.2. The slope was statistically greater than one, but the intercept value was not significant. In terms of deciview, the intercept was statistically greater than zero, while the slope was not statistically different from one (**Figure 8**). On average, measured b_{ext} tended to be higher than reconstructed values by about 2.3 dv .

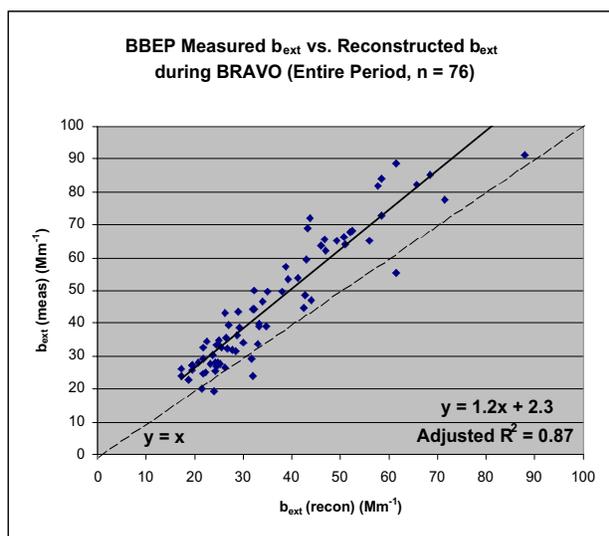


Figure 7 – BBEP Correlation (dv)

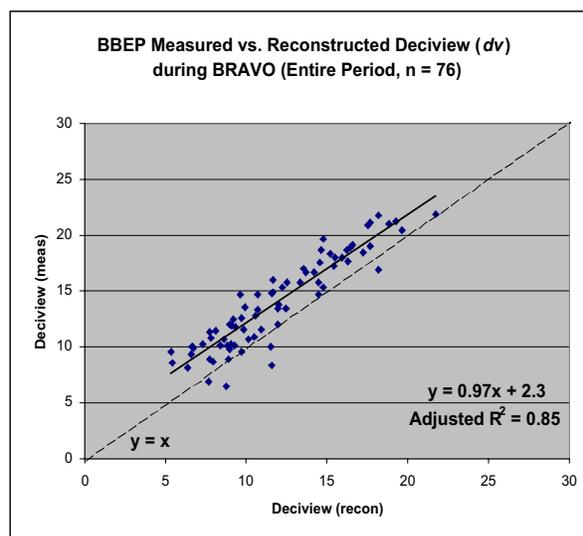


Figure 8 – BBEP Correlation (Mm^{-1})

As the transmissometer lamp ages, light intensity decreases. Transmitters attempt to correct the problem by adjusting applied lamp voltage; however, current lamp properties and feedback design actually translate into light intensity increases over time. All BRAVO b_{ext} data were corrected for this tendency using an average 1 percent per 500 hours lamp brightening function (J. Molenaar, personal communication, August 9, 2001).

Additional lamp brightening adjustments (on top of the default) were made to the BBEP optical data set by other BRAVO researchers (W. Malm, personal communication, November 13, 2002). The same adjustments were applied to BBEP hourly data (subtracted 3 Mm^{-1} for Julian days 193-235, subtracted 7 Mm^{-1} after those dates), and the correlation was reexamined. **Figures 9 and 10** show the correlations of b_{ext} and dv values after lamp brightening adjustments. R^2 values were around 0.88, and the slope was statistically greater than one in both cases. The intercept was instead less than zero (significantly when dv units were used), which meant measured values in the lower ranges ($<13 \text{ } dv$, $<35 \text{ Mm}^{-1}$) were often over-predicted by the reconstruction equation, while the opposite was true for higher ranges. The TCEQ did not have lamp voltage data to determine if additional brightening adjustments were appropriate for BIBE1 data.

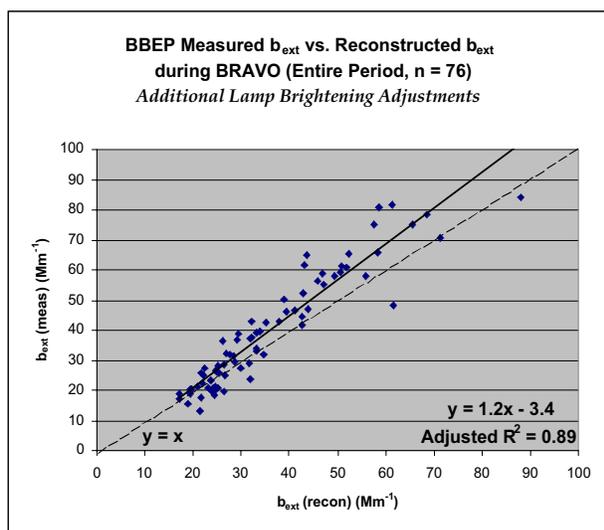


Figure 9 – BBEP Correlation (Mm^{-1}), Additional Lamp Adjustments

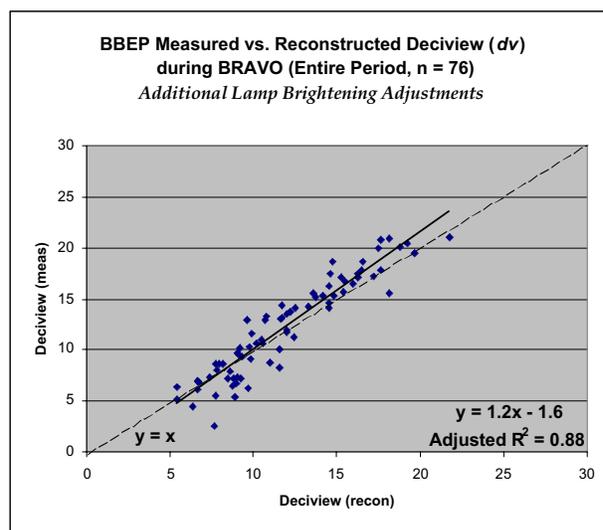


Figure 10 – BBEP Correlation (dv), Additional Lamp Adjustments

BRAVO research focused on characterizing coarse aerosol in west Texas has identified the potential for underestimating coarse particulate scattering in the current reconstruction equation (Malm et al., 2001). This discrepancy could explain some of the biases observed in this report. Also, because nitrates appear to be present as sodium nitrate, rather than ammonium nitrate, scattering efficiency and growth factors in the reconstruction equation for this component may need revision. Continued work in these areas will be helpful in achieving closure between measured and reconstructed b_{ext} at Big Bend. **Table 4** summarizes regression coefficients for both BIBE and BBEP transmissometer versus reconstructed b_{ext} comparisons. Uncertainties noted for the slope and intercept are the 95 percent confidence intervals.

Table 4 – Summary of Regression Results from Measured vs. Reconstructed Light Extinction during BRAVO

<i>Adjustments?</i>	<i>No Adjustments</i>		<i>No Adjustments</i>		<i>Add'l Lamp Adjustments</i>	
<i>Parameter/ Site</i>	BIBE (Mm⁻¹)	BIBE (dv)	BBEP (Mm⁻¹)	BBEP (dv)	BBEP (Mm⁻¹)	BBEP (dv)
Slope	1.2 ± 0.1	1.0 ± 0.1	1.2 ± 0.1	0.97 ± 0.09	1.2 ± 0.1	1.2 ± 0.1
Intercept	1.4 ± 3.7	1.9 ± 0.9	2.3 ± 4.1	2.3 ± 1.2	-3.4 ± 3.8	-1.6 ± 1.2
Adj. R²	0.89	0.91	0.87	0.85	0.89	0.88

Fitting factor scores to b_{ext} data from BBEP (adjusted) had similar results to BIBE1, but not the same. **Table 5** shows that in the summer, the F_1 and F_2 terms were again significant predictors of b_{ext} . While including the CM term increased the R^2 value to 0.89 (but still with a negative coefficient), that variable could not be considered significant at the 0.05 level ($p > F = 0.07$). It may seem odd that dropping the CM term would change the R^2 so much, but without the limitation of so many missing PM_{10} data, the regression picked up nearly twice the number of summer days (46 instead of 24). This does not mean CM was not important to visibility in July and August; in fact, periods with increased coarse particle volume concentration were associated with Saharan dust episodes in these months (Hand et al., 2001). Given the term's strong relationship to sulfates (and F_2) in July-August, some of coarse mass' effects may be incorporated into the F_2 term (or even to some extent, in F_1). Regardless of CM's interaction with the other variables, the soil-related and sulfate-related factors (which also included loadings from species such as nitrates, elemental carbon, and organics) explained about 74 percent of the variance in b_{ext} in the summer. The same variables (without CM) explained about 70 percent of the variance in b_{ext} for this season at BIBE1.

Table 5 – Multiple Regression Fits of Factor Scores and CM to BBEP Daily Average b_{ext}

Season	No. of Days	Adj. R²	Std. Dev. of Error	Resulting Equation
<i>Summer</i>	46	0.74	7.6	$b_{\text{ext}} = 42.6 + 2.6(\text{fRH} * F_1) + 13.9(F_2)$
<i>Fall</i>	55	0.88	7.0	$b_{\text{ext}} = 34.5 + 12.5(\text{fRH} * F_2) + 4.5(F_3) + 2.6(F_5)$

In the fall, the sulfate-related, nitrate-related, and smelting-related factors together explained about 88 percent of the variance in b_{ext} . Interestingly, the CM term could be used in place of the F_3 (smelting) term to achieve the same R^2 value (CM and F_3 were moderately correlated in the fall period, with an $R^2 = 0.45$), but in the above equation, all the terms are assured to be uncorrelated. In comparison, these same three terms achieve an R^2 of 0.87 with BIBE1 data for the same period (adding CM and F_4 explained only 2 percent more of the variance in b_{ext} measurements there).

Back in **Table 3**, differences with the BIBE1 analysis are apparent. For example, the factor associated with organic and elemental carbons (F_4) was not significant in the fall model for BBEP. The most notable difference is that the CM term was not significant in either model for BBEP. Coarse mass was undoubtedly important, but its relationship with some of the other

factors made its role ambiguous. Unfortunately, limited PM₁₀ data prevented its inclusion in factor analysis, and so it is difficult to speculate how CM (or specific PM₁₀ species) would have loaded onto these factors. However, other BRAVO work did assess coarse mass composition from late August through October (Hand et al., 2001) and offers clues, at least for the fall period. Hand et al. found the following components contributed to coarse composition: soil (~40 percent), organic carbon (~30 percent), sulfates (~20 percent), sodium nitrate (~7 percent), and elemental carbon (~2 percent).

Despite differences between BIBE1 and BBEP, these equations do demonstrate that PM-fine sources explain most of variance in b_{ext} data at both transmissometers during BRAVO, and that these sources were associated with many of the components in the reconstruction equation. In the summer, these sources were linked to soil- and sulfate-related factors, and in the fall, to sulfate-, nitrate-, and smelting-related factors. Coarse mass was related to some of these same PM-fine sources and probably explains additional variance in b_{ext} , but its scattering contribution was difficult to identify in this regression analysis. In both periods of the Study, sulfate-related F_2 (possibly partially attributable to coal combustion) explained most of the variance in measured light extinction: 66-69 percent in the summer and 79-84 percent in the fall.

Considering Meteorology

How are these results affected by meteorology, and are they representative of historical conditions at the park? Because higher relative humidity can significantly increase visibility impairment from sulfates at Big Bend, RH conditions should be considered. Ashbaugh et al. determined humidity-induced particle growth was substantial during the mid-September sulfate episode but not significant for other BRAVO episodes (Ashbaugh et al., 2001). This is perhaps one reason F_2 could be used without the $f(\text{RH})$ multiplier in the summer models, while $f(\text{RH}) \cdot F_2$ was the best choice in the fall. Comparing historical meteorological data from 1994-98 to the BRAVO period, the TCEQ determined monthly average RH was lower in July 1999 and higher in August and October 1999, though the variability observed in this parameter during the Study was generally typical of the park (B. Georgoulias, 2003). It is likely then that differences in historical RH impact on visibility were moderated by similar variations during BRAVO, but it would be necessary to examine particular episodes.

Sources are often associated with specific regions, which highlights the importance of wind direction. In general, monthly surface wind patterns during BRAVO were typical when compared to 1995-98 (B. Georgoulias, 2003), offering some evidence that sources affecting the park during the Study were probably the same as in previous years. However, surface winds are not always consistent with upper level transport winds; procedures such as back trajectory analyses should be used to consider wind patterns at higher altitudes.

Conclusion

While reconstructed b_{ext} showed a strong correlation with daily mean b_{ext} during both summer and fall months of BRAVO, measured b_{ext} tended to be higher. On average, the difference between the two values was between 1-2 dv . The BBEP transmissometer measurements showed a similarly strong correlation during the Study period, as well as an average positive offset of 2-3 dv when compared to reconstructed values. When additional lamp brightening adjustments were made to BBEP data, reconstructed b_{ext} tended to overestimate measured b_{ext} in lower ranges and underestimate it at higher values. In all cases, R^2 values were 0.85 or above. Potential improvements to the reconstruction equation include increasing the coarse matter scattering contribution and better characterizing nitrate species' scattering and growth, based on sodium

nitrate properties.

Multiple regression fits of measured b_{ext} to equation components did not produce coefficient estimates that were consistent with the literature; however, collinearity between variables prevented accurate estimates and required another approach. Exploratory factor analysis offered an alternative to reconstructing b_{ext} without the problem of multicollinearity among PM-fine components, and for the most part, regression fits were comparable to using the reconstruction equation. Because factor score estimates and equations were specific to the BRAVO data set, this method did not result in a “new reconstruction equation” for Big Bend. Factor analysis was merely another way of breaking down the components that influenced b_{ext} during BRAVO, as well as providing some insight into the sources impacting visibility at the park in 1999.

This analysis identified five underlying factors, with the two strongest factors related to soil materials and sulfates (coal combustion). Results also suggested influence from metal smelting. Regression analysis linked soil and sulfate factors to measured b_{ext} in the summer, while in the fall, sulfate-, nitrate-, and smelting-related factors explained most of the variance in optical data. It is likely coarse mass also contributed significantly to light scattering during the Study, but hampered by deficient PM_{10} data, this approach could not adequately relate CM to measured b_{ext} along with the factors identified in BRAVO PM-fine data.

Future Work

This analysis grouped factor scores by season. If feasible, a next step would be to group factor scores according to where back trajectories originated and repeat the linear regression analysis with measured light extinction during BRAVO. This approach could help identify regions of particular source-types influencing the park during the Study, but may be complicated by the fact that factor analysis was performed for the entire period (not subsets grouped by transport patterns), and factors were not necessarily entirely related to air mass history.

The TCEQ is currently planning a project to study aerosol characteristics such as particle distribution, coarse mode contribution, and hygroscopic growth properties specific to the Big Bend region throughout the year and compare findings to assumptions of the reconstruction equation. This work is intended to help achieve closure between reconstructed and optically measured b_{ext} , while also enhancing understanding of seasonal variations in PM at the park. The TCEQ will also consider applying factor analysis to historical PM data from the IMPROVE network at Guadalupe Mountains National Park and relating scores to valid optical data collected there.

Disclaimer

The results, findings, and conclusions expressed in this paper are solely those of the authors and are not necessarily endorsed by the management, sponsors, or collaborators of the BRAVO Study. A comprehensive final report for the BRAVO Study is anticipated in 2003.

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Appendix A1.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Initial Factor Method: Principal Factors

Prior Commuality Estimates: SMC									
PNA	PAL	PSI	PS	PK	PCA	PTI	PV	PCR	PMN
0.60171564	0.99121469	0.99615419	0.98371257	0.97428944	0.93230469	0.94719848	0.50750014	0.18305579	0.63856140
FE	NI	CU	ZN	AS	PB	SE	BR	RB	SR
0.99310974	0.31584886	0.32307822	0.78662146	0.49749024	0.70859018	0.64366651	0.77057764	0.61020154	0.91106509
H	NO2	NO3	SO4	NAION	NH4	KION	MGION	CAION	O1
0.98477330	0.26647856	0.82580989	0.96824755	0.80631940	0.97313809	0.63006784	0.50664210	0.72219217	0.70595276

O2	O3	O4	OP	E1	E2	E3
0.88359025	0.71746820	0.84837482	0.95211672	0.96276703	0.83185850	0.64831269

Eigenvalues of the Reduced Correlation Matrix: Total = 27.5500664 Average = 0.74459639				
	Eigenvalue	Difference	Proportion	Cumulative
1	10.8776003	3.7383789	0.3948	0.3948
2	7.1392214	4.6454071	0.2591	0.6540
3	2.4938143	0.8076839	0.0905	0.7445
4	1.6861305	0.3335072	0.0612	0.8057
5	1.3526232	0.3818708	0.0491	0.8548
6	0.9707524	0.2060182	0.0352	0.8900
7	0.7647342	0.0254065	0.0278	0.9178
8	0.7393277	0.1979027	0.0268	0.9446
9	0.5414250	0.0906381	0.0197	0.9643
10	0.4507870	0.0445687	0.0164	0.9806
11	0.4062182	0.1079844	0.0147	0.9954
12	0.2982339	0.0741976	0.0108	1.0062
13	0.2240363	0.0564194	0.0081	1.0143
14	0.1676169	0.0349257	0.0061	1.0204
15	0.1326912	0.0190226	0.0048	1.0252
16	0.1136687	0.0394823	0.0041	1.0294
17	0.0741864	0.0240712	0.0027	1.0321

Appendix A1.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Initial Factor Method: Principal Factors

Eigenvalues of the Reduced Correlation Matrix: Total = 27.5500664 Average = 0.74459639				
	Eigenvalue	Difference	Proportion	Cumulative
18	0.0501152	0.0220685	0.0018	1.0339
19	0.0280467	0.0032006	0.0010	1.0349
20	0.0248460	0.0129652	0.0009	1.0358
21	0.0118808	0.0049707	0.0004	1.0362
22	0.0069101	0.0083798	0.0003	1.0365
23	-0.0014697	0.0033746	-0.0001	1.0364
24	-0.0048443	0.0060501	-0.0002	1.0362
25	-0.0108944	0.0037783	-0.0004	1.0358
26	-0.0146727	0.0072630	-0.0005	1.0353
27	-0.0219358	0.0124705	-0.0008	1.0345
28	-0.0344063	0.0101059	-0.0012	1.0333
29	-0.0445122	0.0146570	-0.0016	1.0317
30	-0.0591692	0.0077704	-0.0021	1.0295
31	-0.0669396	0.0152776	-0.0024	1.0271
32	-0.0822172	0.0083852	-0.0030	1.0241
33	-0.0906024	0.0177081	-0.0033	1.0208
34	-0.1083105	0.0165553	-0.0039	1.0169
35	-0.1248658	0.0157874	-0.0045	1.0123
36	-0.1406532	0.0586538	-0.0051	1.0072
37	-0.1993070		-0.0072	1.0000

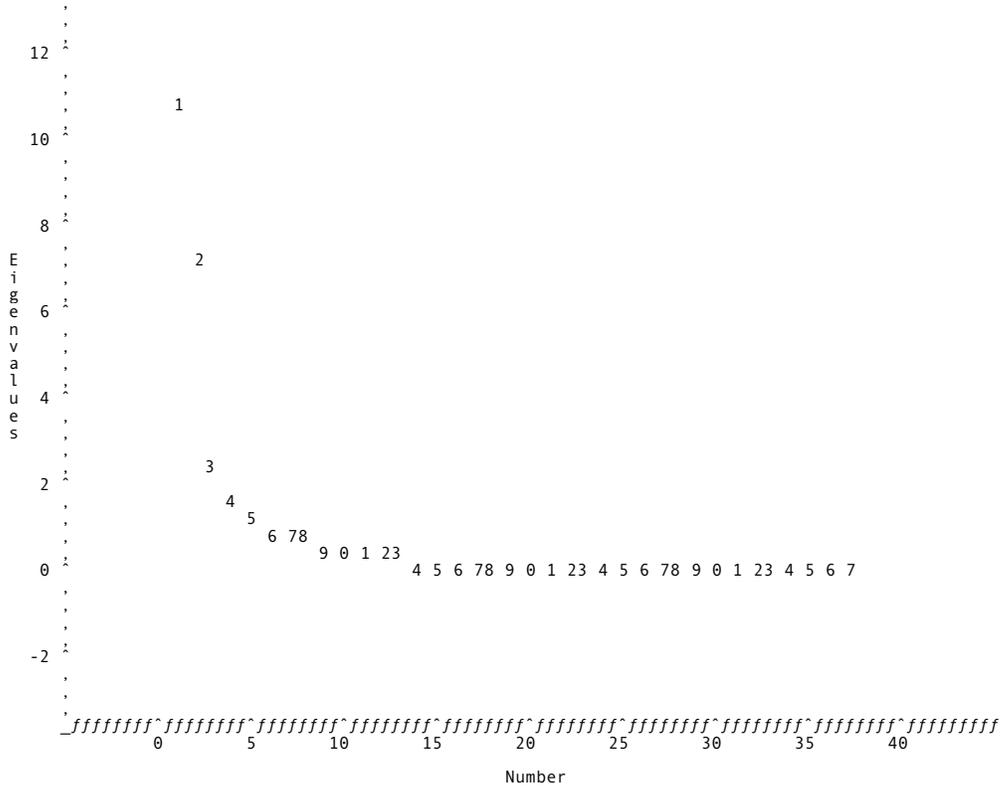
5 factors will be retained by the NFACTOR criterion.

Appendix A1.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Initial Factor Method: Principal Factors

Scree Plot of Eigenvalues



Appendix A1.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Initial Factor Method: Principal Factors

		Factor Pattern				
		Factor1	Factor2	Factor3	Factor4	Factor5
PNA	PNA	40 *	3	-23	24	8
PAL	PAL	79 *	-56 *	-1	-14	9
PSI	PSI	82 *	-54 *	2	-12	9
PS	PS	46 *	76 *	2	-25	27
PK	PK	89 *	-36 *	19	5	3
PCA	PCA	82 *	-40 *	23	6	0
PTI	PTI	83 *	-34	-1	-31	14
PV	PV	22	-32	36 *	-27	-22
PCR	PCR	-10	7	-12	6	14
PMN	PMN	63 *	-26	19	-22	0
FE	FE	82 *	-53 *	2	-12	8
NI	NI	6	4	-19	18	20
CU	CU	-4	24	34	5	1
ZN	ZN	37 *	35	64 *	15	-14
AS	AS	27	21	9	7	23
PB	PB	31	18	58 *	8	-25
SE	SE	27	56 *	-8	-11	32
BR	BR	50 *	49 *	32	31	6
RB	RB	58 *	-44 *	11	-15	-2
SR	SR	77 *	-43 *	-13	11	18
H	H	54 *	72 *	11	-29	22
NO2	NO2	-1	10	13	19	8
NO3	NO3	70 *	-9	-22	51 *	13
SO4	SO4	46 *	76 *	-8	-23	20
NAION	NA_ION	57 *	-21	-40 *	35	23
NH4	NH4	43 *	79 *	-3	-21	16
KION	K_ION	51 *	22	10	40 *	1
MGION	MG_ION	51 *	-39 *	4	-8	5
CAION	CA_ION	65 *	-22	12	30	-15
O1	O1	38 *	-27	-7	-31	-32

Appendix A1.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Initial Factor Method: Principal Factors

Factor Pattern									
		Factor1		Factor2		Factor3		Factor4	Factor5
O2	O2	61	*	53	*	-28		-12	-31
O3	O3	50	*	27		3		23	-38
O4	O4	48	*	69	*	7		17	-15
OP	OP	65	*	51	*	-25		-15	-28
E1	E1	42	*	81	*	-7		3	-20
E2	E2	53	*	15		-58	*	-4	-29
E3	E3	27		-11		-61	*	-1	-27

Printed values are multiplied by 100 and rounded to the nearest integer.
Values greater than 0.356783 are flagged by an '*'.

Variance Explained by Each Factor				
Factor1	Factor2	Factor3	Factor4	Factor5
10.877600	7.139221	2.493814	1.686130	1.352623

Final Community Estimates: Total = 23.549390									
PNA	PAL	PSI	PS	PK	PCA	PTI	PV	PCR	PMN
0.27723079	0.96421065	0.97863282	0.93090792	0.95711601	0.89405114	0.91718825	0.40181317	0.05044425	0.54825716
FE	NI	CU	ZN	AS	PB	SE	BR	RB	SR
0.97561555	0.11187469	0.17449404	0.71160820	0.18577350	0.53188155	0.50843814	0.69761102	0.57045809	0.82791713
H	NO2	NO3	SO4	NAION	NH4	KION	MGION	CAION	O1
0.94314949	0.06700550	0.81363520	0.89515866	0.70364079	0.88994526	0.48866647	0.42034298	0.59448428	0.41999162

O2	O3	O4	OP	E1	E2	E3
0.83325647	0.52307177	0.76176158	0.84829596	0.88871091	0.71632668	0.52642202

Appendix A2.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Rotation Method: Varimax

Orthogonal Transformation Matrix					
	1	2	3	4	5
1	0.79011	0.41610	0.28345	0.31294	0.15592
2	-0.56077	0.76453	0.28974	0.13001	0.01370
3	0.13263	-0.01875	0.60471	-0.61374	-0.48961
4	-0.17201	-0.37993	0.61588	0.04951	0.66656
5	0.11869	0.31250	-0.30121	-0.71137	0.53990

Appendix A2.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Rotation Method: Varimax

		Rotated Factor Pattern						
		Factor1	Factor2	Factor3	Factor4	Factor5		
PNA	PNA	24	13	10	22	38	*	
PAL	PAL	97	*	-2	-5	11	8	
PSI	PSI	98	*	0	-1	10	7	
PS	PS	1	96	*	12	2	5	
PK	PK	92	*	8	28	9	9	
PCA	PCA	90	*	1	29	7	5	
PTI	PTI	91	*	25	-10	11	0	
PV	PV	42	*	-12	9	-5	-44	*
PCR	PCR	-13	4	-8	-4	15		
PMN	PMN	71	*	14	8	4	-15	
FE	FE	98	*	0	-1	11	7	
NI	NI	-1	5	-3	1	33		
CU	CU	-12	14	29	-19	-13		
ZN	ZN	14	31	73	*	-13	-22	
AS	AS	12	32	17	-10	17		
PB	PB	18	15	61	*	-5	-31	
SE	SE	-5	68	*	3	-3	19	
BR	BR	12	48	*	65	*	0	17
RB	RB	75	*	-4	2	6	-8	
SR	SR	83	*	1	3	14	35	
H	H	11	95	*	18	3	-4	
NO2	NO2	-7	3	20	-11	10		
NO3	NO3	50	*	7	31	28	62	*
SO4	SO4	-1	93	*	10	14	8	
NAION	NA_ION	48	*	2	0	25	64	*
NH4	NH4	-5	92	*	16	13	4	
KION	K_ION	23	23	52	*	14	31	
MGION	MG_ION	64	*	-4	0	4	3	
CAION	CA_ION	58	*	-6	42	*	22	16
O1	O1	46	*	-3	-11	34	-29	

Appendix A2.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Rotation Method: Varimax

Rotated Factor Pattern								
		Factor1	Factor2	Factor3	Factor4	Factor5		
O2	O2	13	61 *	18	64 *	0		
O3	O3	16	21	50 *	45 *	1		
O4	O4	-5	61 *	53 *	31	8		
OP	OP	19	63 *	17	62 *	-1		
E1	E1	-16	72 *	39 *	43 *	3		
E2	E2	23	27	-10	74 *	18		
E3	E3	16	-4	-25	63 *	19		

Printed values are multiplied by 100 and rounded to the nearest integer.
Values greater than 0.356783 are flagged by an '*'.

Variance Explained by Each Factor						
	Factor1	Factor2	Factor3	Factor4	Factor5	Total (A1., p.2)
	9.1484255	6.4325873	3.1475038	2.8138732	2.0070000	27.55
% of Total Variance	33.2 %	23.3%	11.4%	10.2%	7.3 %	85.4%

Final Community Estimates: Total = 23.549390									
PNA	PAL	PSI	PS	PK	PCA	PTI	PV	PCR	PMN
0.27723079	0.96421065	0.97863282	0.93090792	0.95711601	0.89405114	0.91718825	0.40181317	0.05044425	0.54825716
FE	NI	CU	ZN	AS	PB	SE	BR	RB	SR
0.97561555	0.11187469	0.17449404	0.71160820	0.18577350	0.53188155	0.50843814	0.69761102	0.57045809	0.82791713
H	NO2	NO3	SO4	NAION	NH4	KION	MGION	CAION	O1
0.94314949	0.06700550	0.81363520	0.89515866	0.70364079	0.88994526	0.48866647	0.42034298	0.59448428	0.41999162

O2	O3	O4	OP	E1	E2	E3
0.83325647	0.52307177	0.76176158	0.84829596	0.88871091	0.71632668	0.52642202

Appendix A2.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Rotation Method: Varimax

Scoring Coefficients Estimated by Regression

Squared Multiple Correlations of the Variables with Each Factor				
Factor1	Factor2	Factor3	Factor4	Factor5
0.99506399	0.98894508	0.93682780	0.92560034	0.89042115

Standardized Scoring Coefficients						
		Factor1	Factor2	Factor3	Factor4	Factor5
PNA	PNA	0.02242	0.00861	0.00250	-0.00511	0.02395
PAL	PAL	-0.02903	-0.11609	0.13990	0.27223	0.18295
PSI	PSI	0.58637	0.33945	-0.82233	-0.46408	-0.66276
PS	PS	0.03710	0.14660	-0.23599	-0.13064	0.70434
PK	PK	-0.01275	-0.13827	0.63066	0.11245	0.13679
PCA	PCA	0.09321	-0.08551	0.19868	-0.00106	-0.01662
PTI	PTI	-0.00882	0.07698	-0.15240	0.02090	-0.00846
PV	PV	0.01757	-0.02407	0.02661	0.02247	-0.06777
PCR	PCR	-0.00691	0.01223	-0.00719	-0.01007	0.04147
PMN	PMN	0.03343	-0.00391	0.01569	0.00823	-0.12022
FE	FE	0.36202	-0.04186	-0.07533	-0.21457	0.13352
NI	NI	-0.01495	-0.00327	0.01156	0.00567	0.04329
CU	CU	-0.00310	0.00618	0.04410	-0.04735	0.00284
ZN	ZN	0.04591	-0.02592	0.24314	-0.03942	-0.19925
AS	AS	-0.00553	0.03433	0.00546	-0.07808	0.08084
PB	PB	-0.01464	-0.05876	0.17181	0.02336	-0.13194
SE	SE	-0.01178	0.03239	-0.02875	-0.04483	0.11034
BR	BR	0.00471	0.05084	0.04781	-0.11770	0.15381
RB	RB	0.01380	-0.00440	-0.00547	0.00045	-0.06033
SR	SR	-0.08482	0.01824	0.03808	0.02104	0.31939
H	H	0.09004	0.45118	0.03823	-0.30417	-0.69717
NO2	NO2	0.00116	0.00862	0.06148	-0.04832	0.00486
NO3	NO3	-0.01611	-0.03081	0.07445	-0.02864	0.43117

Appendix A2.

Factor Analysis of BRAVO PM-fine Data from Big Bend 12-hr and 24-hr Sites

The FACTOR Procedure Rotation Method: Varimax

Standardized Scoring Coefficients						
		Factor1	Factor2	Factor3	Factor4	Factor5
SO4	SO4	0.08320	0.19163	-0.24939	-0.11080	0.09656
NAION	NA_ION	0.00466	-0.04270	0.04741	0.07409	0.26420
NH4	NH4	-0.06303	0.25923	-0.05280	-0.08482	-0.15049
KION	K_ION	0.00763	-0.02209	0.02703	-0.01653	0.14269
MGION	MG_ION	0.02186	-0.02587	0.03288	0.02216	-0.03758
CAION	CA_ION	0.02813	-0.03494	0.08684	0.02800	-0.03263
O1	O1	0.01275	0.01104	-0.04812	0.11018	-0.06060
O2	O2	0.02429	-0.03142	-0.02620	0.36098	-0.17640
O3	O3	0.00193	0.00820	0.06125	0.05053	-0.06919
O4	O4	-0.07563	-0.07932	0.23919	0.18711	0.00134
OP	OP	-0.05917	0.08072	-0.14598	0.35027	-0.13957
E1	E1	-0.08967	-0.01158	0.40586	0.12039	0.06649
E2	E2	-0.03163	-0.07393	-0.01033	0.32757	0.03395
E3	E3	-0.00133	0.00388	-0.11028	0.13770	-0.01338