5. Assessment Approaches

5.1 Overview

Assessment includes all systematic uses of data and other information to meet the BRAVO Study objectives. Some of the assessment methods provide results that directly address one or more of the study objectives, while others provide information useful or required as intermediate results in the overall process of assessment. Among the latter reasons for assessment is to check the plausibility of the data (i.e. a form of data validation) and to familiarize data analysts with conditions in the study region. The assessment approaches that will be used range from very simple data summary and display methods that are applied to parameters one at a time to sophisticated models that require dozens of parameters and numerous assumptions.

A major product of the BRAVO Study is the development of a conceptual model of the important physical and chemical processes that are responsible for haze conditions in Big Bend National Park. The conceptual model is a plausible descriptive explanation of the causes of impairment that is supported by the measurement data. It includes the identification of the important sources (i.e., individual major sources, source types, and source areas), and a description of the meteorological conditions under which these sources contribute to Big Bend haze. Case study analyses are narrative histories of individual haze episodes that illustrate the measured and modeled components of a conceptual model.

Attribution analyses are quantitative assessments of the contributions by important sources. Attribution methods are typically divided into two broad categories: predictive air quality models and receptor models. Air quality models use meteorological measurements, pollutant emissions data, and calculated or assumed boundary conditions to calculate the transport, dispersion, deposition and chemical transformation of pollutants emitted into the atmosphere at specific known emission source locations. Receptor models rely on the ambient air quality measurements made at monitoring site and the characteristics of the likely emission sources to infer the contribution of those sources. Another category of attribution analysis is a hybrid of these. For example a wind field model could indicate the transport path of the pollutants measured at a site and receptor methods used to apportion among the sources along that path, or a unique tracer for a source (a receptor method) could be used to determine the transport and dispersion of primary pollutants while production of the secondary aerosol is estimated with the atmospheric chemistry portion of an air quality model.

One of the design strengths of the BRAVO Study is the planned use of multiple attribution analyses methods. Comparisons of results from various attribution methods that utilize different assumptions and data sets can provide insights not otherwise achievable by any single attribution method. If the results tend to agree, credibility is enhanced. If they are inconsistent, a reconciliation process is applied which may uncover inappropriate model assumptions or questionable input data, or in the worst case be used

to determine a suitable range of uncertainty for the study findings. A corollary to the use of multiple attribution methods is the involvement of multiple individual data analysts/modelers often working for different organizations. Generally, those who conduct the analysis or modeling are proponents of the methods they apply who champion them in an almost competitive atmosphere that drives them to do all they can to make their approach successful. In other words experts motivated to have them succeed vigorously apply each method.

Of the various attribution methods that will be applied, only regional air quality modeling can be used to address all of the important emission sources in the region for any time period, including times outside of the BRAVO Study period. A major product of the study is the evaluation, and fine-tuning (if needed) of a regional air quality model for uniform application to all of the important emission sources in the region. The reconciliation process will determine if air quality modeling produces results that are consistent with the best of the other methods and if not whether they can be made more consistent by modifying the assumptions within acceptable ranges or changing which input data are utilized. The best of the regional air quality models that are evaluated in the BRAVO Study will be applied to all of the important emission sources as a means to ensure consistent evaluation of each source's contribution to haze at Big Bend.

The remainder of this section of the plan is organized into subsections by the types of assessment methods, beginning with the simple descriptive assessment and ending with the development of overall BRAVO Study findings as a result of the reconciliation process.

5.2 Descriptive Analysis

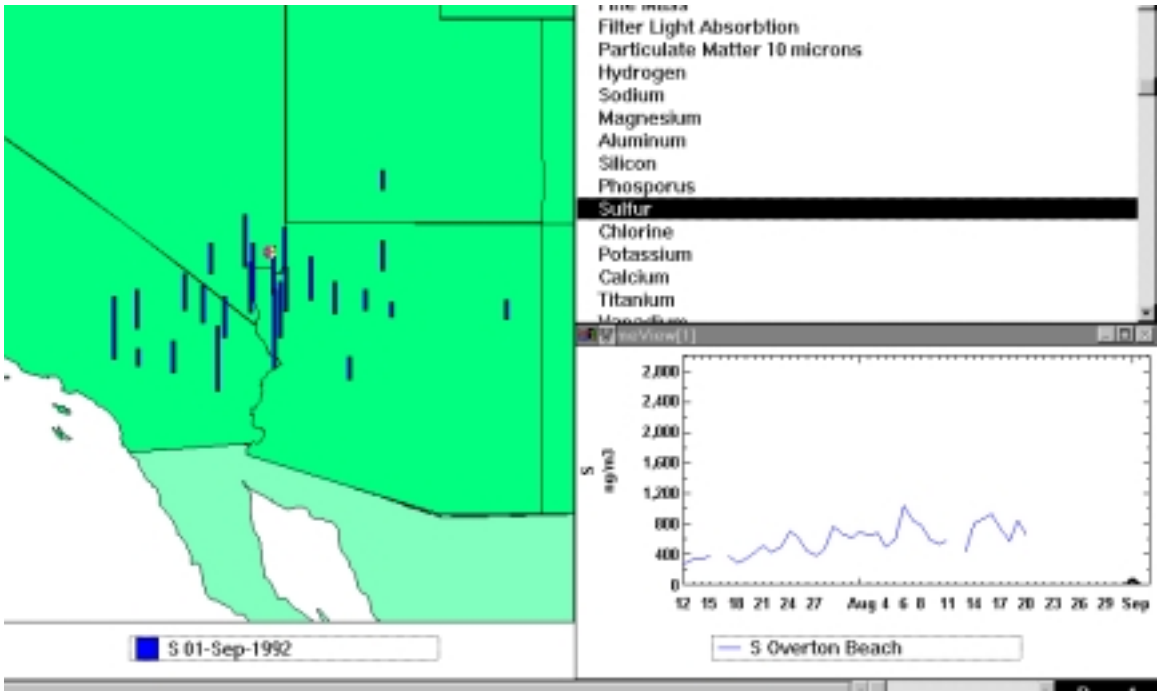
Several purposes are served by descriptive analysis including data quality assurance and validation, data familiarity, and a means of testing the plausibility of some aspects of prospective conceptual models.

The initial steps in determining data quality assurance and validation are the primary responsibility of the organizations that made the measurements. These usually include checking for outliers (values beyond physical or typical limits), and spatial and temporal trends that are too large to be believed (maps of data values by time period, and time plots or limits on a change from one period to the next). Data with substantial inconsistencies are then the subject of further investigation to attempt to identify the cause, correct the data if possible and flag it if necessary.

The measurement organizations are fully responsible for the first of these three activities, and often will conduct some of the second and third activities. Independent data analysts will supplement the activities of the data collection organizations were necessary to look for suspect data based upon unlikely spatial and temporal trends. It is essential that all measurement organizations identify the data validation steps that they intend to conduct so that others can apply the required additional validation steps. Data

will not be submitted to the database until it has reached validation level 1A (see discussion of data validation levels in section 6.4).

The enormous amount of data collected in a study like BRAVO makes the use of summary statistics and displays essential for the analysts to gain familiarity with it. Data analysts will want to become familiar with those subsets of the data that they intend to use or that may be pertinent to the conceptual model that justifies the assessment methods they are promoting. While data analysts will have the ability to download any data they wish and apply their favorite statistics and graphics programs, a specific set of data summary tables and display figures will be provided to all of the analysts to minimize duplicative efforts. To further facilitate efficient familiarization with the data, many of the key ambient measurement values (e.g. aerosol species, major components & mass, tracer concentration, optical parameters, wind data, etc.) will be put into Voyager™ format so that spatial maps and time plots of the data can be very quickly generated by the analysts using the Voyager™ program. Figure 5-1 shows an example of a VOYAGER data plot from Project MOHAVE.



Example VOYAGER data plot from Project MOHAVE. The map view shows relative particulate sulfur concentrations for September 1, 1992. The time series plot shows sulfur concentrations each day of the study for an individual site. By clicking on another site on the map, time series is then shown for that site. Similarly, by clicking on another day on the time series, the map shows the spatial pattern for that day. Finally, clicking on another variable in the variable list changes the variable that is mapped and shown as a time series.

Often a data analyst recognizes a significant aspect of the data that was not noticed by the other analysts. To promote the sharing of these often-important insights, frequent (e.g. quarterly) data analysis meetings will be scheduled with briefing by all of

the active data analysts. Email and other telecommunications will be promoted between the data analysis meetings to ensure timely sharing of information.

A primary means of testing the credibility of a conceptual model is by determining if it is consistent with the validated data. Experienced data analysts in the initial stages of a complex study such as BRAVO bring to the study a number of possible simple conceptual models based upon findings in earlier studies. Much of the process of data familiarization is in fact informal checking of consistency between the possible conceptual models and the data. When an analyst indicates that the data seem reasonable or makes sense, in fact he (she) is indicating that it fits satisfactorily with some elements of a conceptual model of the important phenomena. For example if the sulfate concentrations are similar over a large areas it confirms the widely held belief that as a secondary component (produced in the atmosphere over many hours) sulfates should be regional in scale. If nearby monitoring sites have at times very different sulfate concentrations, one or more of the sites might be impacted by a source of primary sulfate emissions (a very different conceptual model for the sulfate source).

Descriptive data analysis methods will also be applied to data from short-term and special studies done as part of or in conjunction with the BRAVO Study. These include any measurements made on a non-routine basis (e.g. microscopy and carbon speciation of select aerosol samples, or relative humidity growth studies) or by mobile platforms (e.g. aircraft measurements). However, the specialized nature of these efforts makes it difficult to include in a general description of assessment analyses. The organizations that conduct these measurements are expected to produce separate reports of their results. They may be asked to provide specific additional data analysis as needed to help in developing or confirming a conceptual model or to provide needed inputs to other assessment methods.

Validation checks will need to be applied to all of the data before they are entered into the database. The timing for data availability in the database will vary depending on the type and source of the data. Generally data generated by subsequent laboratory analysis of samples collected at monitoring locations (e.g. particle filter samples and tracer samples) will require longer than instrumentally measured data (e.g. optical and meteorological data). The former may not be all incorporated into the database before the end of March 2000, while the latter may be available by the end of December 1999. Except for data validation checks, most of the analyses will not be applied to data prior to its availability in the BRAVO Study database.

Table 5-1 summarizes the various descriptive analysis methods, the data they will be applied to and which organization are responsible for conducting the analyses.

Table 5-1. Application of descriptive analyses methods to various data types and the organizations responsible for conducting the analysis.

Analysis Methods Types of data	Validation checks	Time plots	Maps by time period	Univariate statistics
Aerosol mass & major components & size dist.	UCD & CSU	CSU	DRI & TNRCC	DRI
Aerosol trace elements (by PIXE & XRF)	UCD & CSU	Voyager™[1]	Voyager™	DRI
Optical data (b_{ext}, b_{scat}, b_{abs})	ARS & DRI	Voyager™	N/A[2]	DRI
Ambient tracer data (24-, 6-, & 1-hour)	BNL & EPRI	DRI	Voyager™	DRI
Tracer emission rates	NOAA-FRD	NOAA-FRD	N/A	DRI
Surface meteorological data (ws, wd, T, & RH)	N/A	Voyager™	Voyager™	DRI
Upper air meteorological data (ws, wd, T, & RH)	NOAA-ETL	DRI	Voyager™	DRI
Annual emission rates – point & area sources	N/A	N/A	DRI	DRI
Continuous emission rates—select point sources	N/A	DRI	N/A	DRI

5.3 Association Analysis

Association analyses are similar to descriptive analyses except that more than one parameter is considered at a time. Like descriptive analysis, association analysis is an important step in data quality assurance and validation, promotes data familiarity, and is a means to test conceptual models. In addition association analysis allows precision (and other quality descriptors) to be directly determined from collocated measurement, permits assessment of aerosol and optical closure at some of the more complete monitoring sites, and may reveal insightful relationships concerning the conditions associated with and causes of haze.

In cases with collocated measurement of the same parameter, measurement approach, and organization a direct determination can be made of data precision, uncertainty, and lower detection limit. Correlation analysis and scatter plots of the paired data are inspected to identify data outliers or systematic differences between the two samplers (e.g. flow inconsistencies). Standard algorithms to calculate precision, uncertainty and detection limits are used (see quality assurance- section 7). Such determinations are the responsibilities of the measurement organizations.

Comparisons of coincident similar measured parameters (e.g. elemental sulfur and sulfate, or use of different samplers or laboratories to obtain nominally the same measurement) can be used to identify periods with outliers and/or systematic

[1] Except for some specifically requested plots, these analyses will not be done centrally but will be left to individual data analysts using Voyager™ or some other graphic/statistics software.
[2] N/A is not applicable or not attainable.

inconsistencies. As with collocated measurements, the usual method is to examine scatter plots and conduct regression analysis. In cases where the related measurements are made by the same organization, they are responsible for the assessments. If the related measurements are by different organizations, another organization will typically do the assessment.

A series of simple closure determinations are possible using association analysis of some of the measurements. In essence, closure is a consistency check involving measured data and simple conceptual models. The following are the principal closure exercises for the BRAVO Study:

- Fine mass closure – compare the sum major of measured species combined with the mass of the assumed common oxides and other non-measured components (ammonium ion for sulfate and nitrates, etc.) with the gravimetric fine mass;
- Optical closure – compare the sum of the measured light scattering and light absorption with the total measured light extinction; and
- Extinction budget – compare the sum of the calculated extinction for the major aerosol components (component concentration multiplied by an extinction efficiency that may be a function of relative humidity) with the measured total light extinction.

The Big Bend monitoring site is the only one with sufficient measurement to check closure for each of these. Comparisons would include scatter plots and regression analysis of the sum of the measured or derived components with the measured total. Time plots of the components and totals are also useful to look for temporal patterns when closure may be a problem (e.g. optical closure problems during a certain time of day might result from sunlight interfering with the transmissometer). Figure 5-2 is an example of fine mass closure from the Project MOHAVE final report. Figure 5-3 is an example of optical closure from Project MOHAVE.

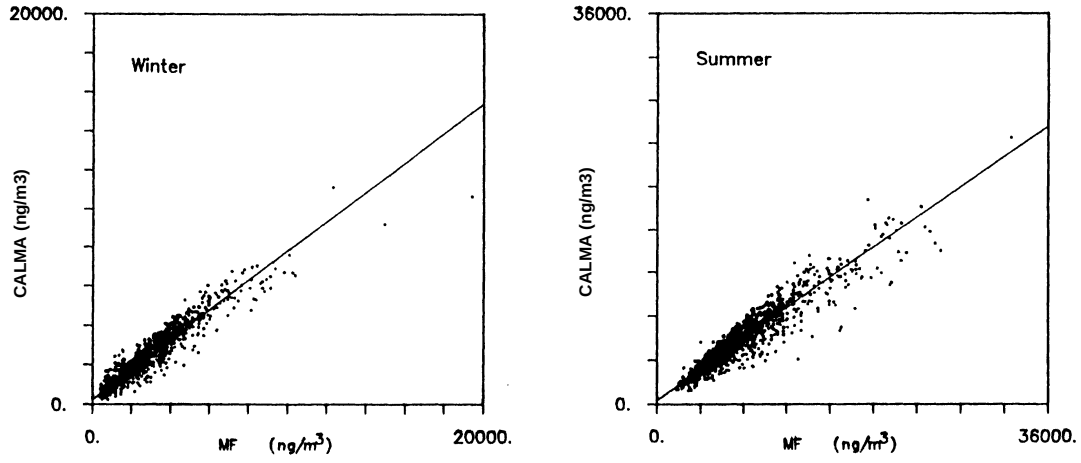


Figure 5-2. Comparison of gravimetric mass (MF) and calculated mass (CALMA) at all Project MOHAVE IMPROVE sites. The left plot is for winter and the right plot is for summer. The slopes are 0.76 (winter) and 0.70 (summer). The correlation coefficients (r^2) are 0.89 (winter) and 0.89 (summer). The number of data pairs are 1102 (winter) and 1533 (summer).

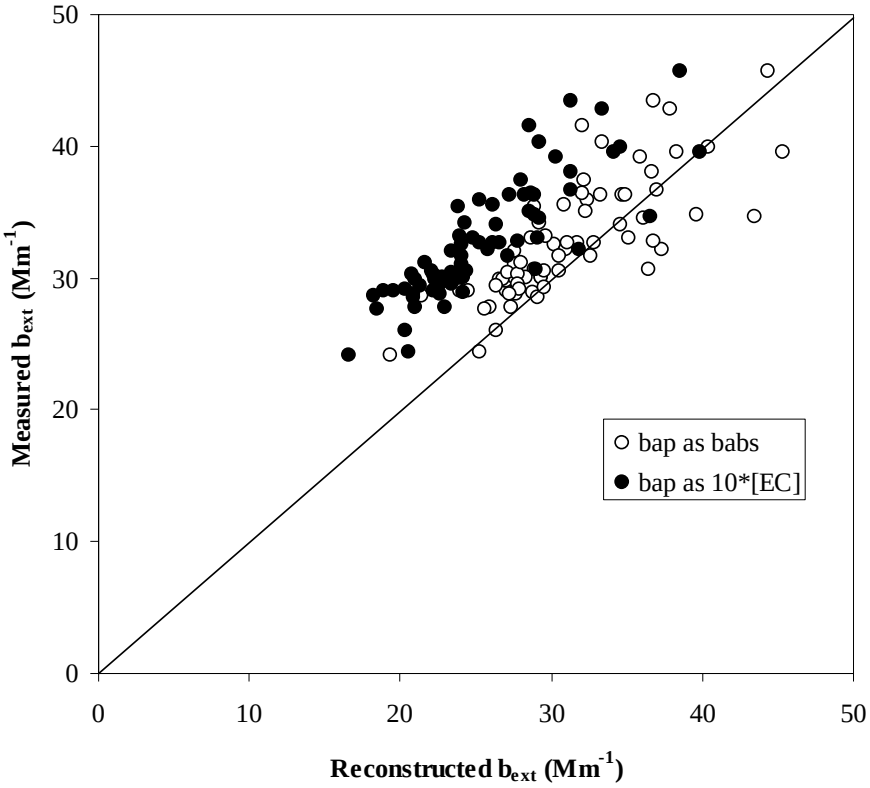


Figure 5-3. Comparison of measured extinction with calculated extinction ($b_{sg} + b_{sp} + CMS/2 + b_{ap}$). The open circles were calculated using $b_{ap} = b_{abs}$. The closed circles were calculated using $b_{ap} = 10$ [EC]. The line is the 1:1 line.

Using association analysis methods data analysts can explore possible relationships between any of the measured parameters to help develop or evaluate conceptual models, to identify the conditions that are conducive to haze events, and to identify the aerosol components that are significant contributors to the haze. For example a positive correlation between the fraction of sulfur that is particulate and the presence of low clouds might indicate that aqueous chemistry is an important mechanism for converting the SO_2 to sulfate during the study. An association between wind speed beyond some threshold and increased soil aerosol component concentration could be used to identify locally suspended dust as a principal source of the soil component. Extinction budget analysis will permit an estimate of the extinction contribution by the major aerosol components for each sample period. Combining these with wind direction in a wind rose analysis could indicate that some aerosol extinction components are enhanced during local flow from certain directions.

There are an incredibly large numbers of possible combinations of data that could be examined for associations for exploratory purposes, most of which would not yield productive results. Experienced data analysts narrow the choices to a manageable effort by having specific conceptual models that they explore in an effort to better understand the important processes for this study. Another approach to narrowing the choices is to reduce the dimensions of the data matrix by any one of several statistical analyses methods known as factor analysis. These include factor analysis, principal component,

eigenvector analysis, and empirical orthogonal function analysis methods. These methods attempt to simplify the description of the system by determining a minimum set of vectors that spans the data space to be interpreted. In other words, a new set of variables is found as linear combinations of the measured variables so that the observed variations in the system can be reproduced by a smaller number of these causal factors.

Table 5-2. Application of association analysis methods (i.e. scatter plots and regression analysis) to various data types and the organizations responsible for conducting the analyses.

Analyses Types of data	Validation checks	Quality assurance parameters	Closure assessment	Exploratory (compare to any data)
Aerosol mass & major components & size dist.	UCD & CSU	UCD & CSU	NPS & UCD	Any analyst
Aerosol trace elements (compare PIXE & XRF)	UCD	UCD	N/A	Any analyst
Optical data (b_{ext}, b_{scat}, b_{abs})	ARS & DRI	ARS & DRI	NPS	Any analyst
Aerosol extinction	N/A	N/A	NPS, UCD	Any analyst
Ambient tracer data (24-, 6-, & 1-hour)	BNL & DRI	BNL, DRI, & EPRI	BNL, DRI, & EPRI	Any analyst

5.4 Study Period Representativeness

In order to know how applicable BRAVO Study results are to other periods of times (other times of the year and other years), the representativeness of the study period must be determined. If the study period is found to be significantly unusual compared to typical years or long-term composite conditions, the results should be interpreted in light of this finding.

The approach used to determine representativeness of the study period starts by comparing meteorological and air quality data during the study period with similar data for other times during the year and for the same period of time in previous years. Simple statistical tests and comparisons of frequency distribution plots for the study period and other periods show the degree of similarity of the study period to those other periods for each parameter. For example, the frequency distribution of the light extinction coefficient at Grand canyon National park for the Project MOHAVE summer (1992) is compared to other years in Figure 5-4. The study period will undoubted be quite different in many respects from other time of the year, since that period was chosen for its association with high haze levels and flows from know emission source areas. However it is not so likely that for many of the parameters this analysis will indicate that the study period was particularly unusual compared to the same period in previous years (because by definition unusual events rarely happen). These preliminary representativeness comparisons can begin as soon as the BRAVO Study data is available in the database.

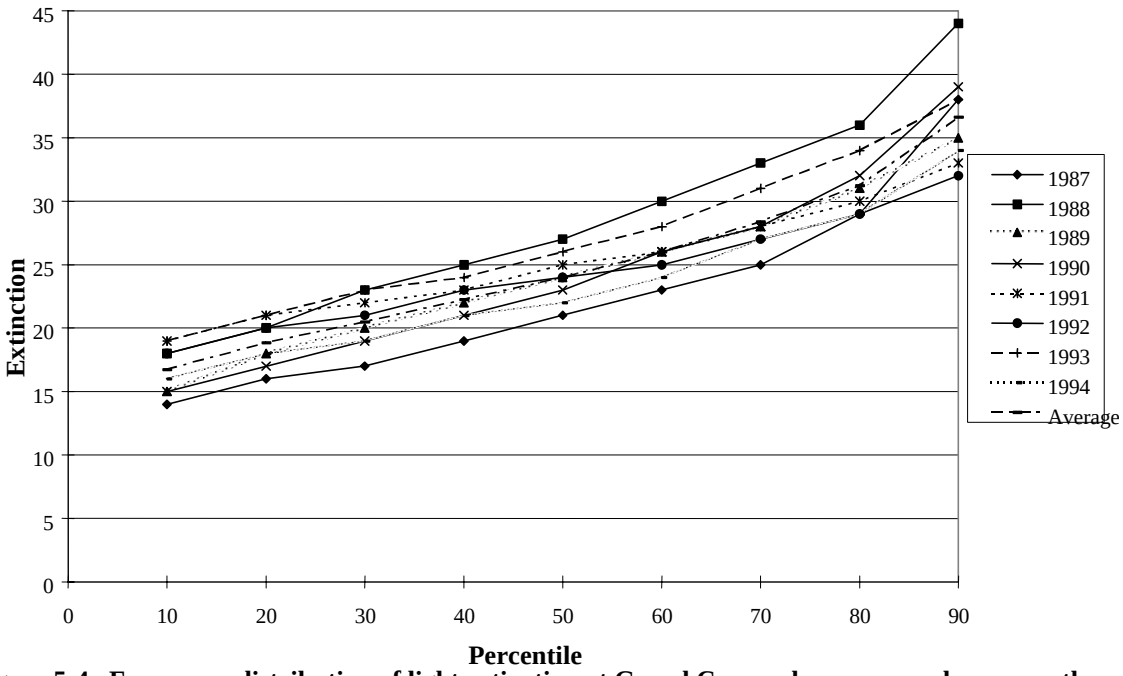


Figure 5-4. Frequency distribution of light extinction at Grand Canyon by season and year: south rim, summer (May – October).

Undoubtedly the frequency distribution for some parameters will be significantly different compared to the corresponding distributions for some of the previous years. The question of how significant these differences are can be best addressed in the context of the conceptual model that will be developed as a major product of the BRAVO Study. For example, the conceptual plan may indicate that sulfate particulate concentrations are much higher when transport is from a specific SO_2 source region if low clouds that promote rapid atmospheric chemistry accompany them. An unusual joint frequency of the two conditions (i.e. clouds and transport from the source region) during the study period would be considered significant to the findings of the study. In this circumstance one would expect unusual sulfate concentration, which would give further support to the validity of the conceptual model. Representativeness comparisons guided by conceptual models must be done towards the end of the data assessment process when conceptual models are well developed.

If significant differences are found between the study period and the same periods in other years, data analysts can attempt to reconstruct the results that might by found in a typical year. This would be accomplished by generating a weighted frequency distribution of study results using the long-term average frequency of conditions to determine the weighting factors. For example, a source area might be found to contribute 5% of the study-periods sulfate, but the study was done in a year where flow from that source region was three times as often as during the long-term average. The contribution could be recalculated with one-third the frequency of impact by that source area and a corresponding increase in the frequency of impacts from the under-represented areas during the study period. The reconstructed contribution by the example source would be much reduced. Another approach that could be used to reconstruct results for a

typical year is to use the most credible of the air quality models with current emissions but using meteorology that is more typical of the long-term average conditions. The steering committee will determine whether there is a need to reconstruct the findings to adjust for unusual study period conditions near the end of the data analysis process.

Desert Research Institute will be responsible for all of the preliminary representativeness analyses. UC-Davis and Colorado State University will also consider the representativeness of aerosol concentrations during the study period. Subsequent work to determine the significance of differences between the study period and other periods, and to reconstruct the results will only be conducted as needed. They may be done by any of the data analyst or modeling organizations depending on the nature of the effort. Data analysis meetings are the appropriate forums for making these decisions.

5.5 Source Attribution

The principal purpose of source attribution analyses is to estimate magnitude, duration, and frequency of visibility impairment at Big Bend by major sources or source categories. These analyses should also result in a better understanding of the conditions and causes of impairment (conceptual models) and some of the methods could subsequently be used to predict the visibility response to emission changes (not considered part of the BRAVO Study).

Attribution assessment is the most difficult of the data assessment tasks, its results are likely to spark the liveliest debates, and it will consume the majority of the BRAVO Study data analysis resources. All source attribution methods require the use of numerous critical assumptions many of which can be reasonably challenged. The practitioners of the various attribution methods are usually strong proponents of their approach while often are highly critical of the capabilities of competing methods. The inner workings of many of the methods range from complex to obscure with the result that it is often difficult for those who are not expert in the method to understand the sensitivity of the results to input data and assumption uncertainties.

Often studies will employ only one attribution method, which has the advantage of minimizing the cost and internal controversy of the assessment results. The disadvantage of the one-method approach is that there may be very vocal external critics of the final study findings who are proponents of alternative approaches. BRAVO Study technical management has chosen to include numerous distinct methods applied by their proponents so that any voices of dissent can be heard at data analysis meetings when there remains time to reexamine, refine, and reapply approaches that are accused of deficiencies. The obvious disadvantage of the multiple-method attribution approach is the additional time and cost required, plus the need for a results reconciliation effort (discussed in the next section) to develop study findings that reflects the overall judgment of the technical committee.

Attribution methods are typically divided into two broad categories: air quality simulation models and receptor models. The first method – receptor data analysis or receptor modeling – is an analysis of concentrations and chemical composition data collected at one or more receptor locations, sometimes in combination with meteorological information, and comparison of the receptor data with the composition of emissions from sources of interest. Receptor modeling is a diagnostic approach that analyzes measurements to derive a plausible accounting of the emissions that produced measured concentrations and compositions. Although conceptually straightforward, receptor modeling depends on accurate measurements of ambient concentrations and, in many cases, on accurate characterization of the compositions of emissions from major source categories. In practice, some receptor analysis methods can be statistically complex. Receptor analysis can only be used to analyze conditions at the times and locations for which measurements exist: it has no predictive capability for other times and locations.

Many receptor methods are also limited to attributing sources for which there are distinctive chemical signatures. Most prior information on emission source composition profiles is from measurements made years ago of sources outside of the study region. The BRAVO Study included a substantial effort to make new measurements of source characteristics from many types of industrial, commercial, transportation, agricultural, and natural sources (section 4.4 summarizes the source types that were included). It was not possible to characterize all of the larger sources in the study region; so composite source profiles by source type will be developed and made available to analysts in the BRAVO Study database.

A fundamental assumption for many receptor model approaches is that the ratio of the species of interest and the unique source characteristic that is used to identify the source is preserved during transport from the source to the receptor sites. This is not the case for sulfate formed in the atmosphere by conversion of SO_2. Hybrid receptor models that add a parametric representation of the chemical conversion and/or deposition processes to the basic receptor model are used to overcome this limitation.

The second method – source emissions simulations or simulation modeling – uses mathematical models of the transport, diffusion, deposition, and chemical conversion of the emitted pollutants to predict ambient concentrations resulting from emissions. Such models, which rely on our understanding of the physics and chemistry of the atmosphere, are conceptually able to predict air quality impacts at all locations and time. Because of limitations in our knowledge of atmospheric behavior, or ability to portray that knowledge mathematically, and the ability of computers to carry out the needed calculations in a reasonable amount of time, all models require some input data on meteorology and air quality, in addition to the obvious requirement of emissions information.

Past mesoscale tracer studies (Project MOHAVE, WHITEX, NGS Study, etc.) have shown that air quality simulation models perform poorly in their ability to predict tracer concentrations in regions dominated by complex terrain. Limited computational

resources force modelers to compromise between the overall domain of the modeled area and the grid size that is considered. Large study regions in complex terrain usually result in modeling that cannot spatially resolve many flow influential terrain features (e.g. canyons, ridge lines, etc). Nested grid models allow modelers to increase the spatial resolution at some locations in the domain. However, for studies like BRAVO where the domain is of the order of a thousand kilometers the smallest grid in a nested model may be of the order of ten kilometers, which is still too coarse to adequately resolve the Rio Grand River Canyon at Big Bend.

The BRAVO Study tracer data will be used to evaluate the performance of both types of attribution models used in the study and will also be available for direct or indirect use to enhance model performance. Air quality simulation models' predictions of the tracer compounds released during the BRAVO Study will be compared to the measured concentrations to evaluate their ability to simulate transport and dispersion. Modelers may change certain aspects of the air quality model (e.g. selection of input data, boundary conditions, etc.) to improve their ability to predict the tracer concentrations. Receptor models that can predict the pollution contribution from sources that have been tagged by tracer can also predict the tracer concentrations by appropriate scaling of the predicted pollution concentration by the ratio of tracer to pollutant release rates. Some receptor models may use the tracer data as input to predict the contribution of the tagged sources and must be evaluated in other ways.

Tracer data will be divided into two subsets by time periods. One of the subsets will be placed in the database relatively early in the assessment phase of the study so that it can be used as input to or to fine-tune attribution models. The second subset will be submitted to the database after the attribution models have been documented and will be used to openly evaluate their performance. Schedules and procedures for subdividing and use of the tracer data will be developed in consultation with the data analysts during data analysis meetings.

Receptor and air quality simulation models that will be used during the BRAVO Study are described below starting with the receptor methods. Most of the methods described were used in Project MOHAVE to assess the particulate sulfate contribution to haze from the Mohave Power Project (MPP). Many of these methods can be adapted to assess primary particulate (e.g. crustal components and soot) and perhaps other secondary particulate (e.g. secondary organics and nitrates).

Tracer Scaling (also called Tracer Max)

Tracer scaling is a simple method employed in Project MOHAVE to determine the maximum possible sulfate that could be associated with tracer tagged sources of SO_2. In that study the ambient PFT data, scaled by the tracer/SO_2 stack emission ratio, were used to deduce the maximum possible Mohave Power Project (MPP) contribution to particulate sulfur at Meadview and Hopi Point (primary receptor sites) if all SO_2 were to be converted to particulate sulfur and there were no deposition losses (Green and Tombach, 2000). Whenever the maximum possible particulate sulfur that was calculated

in this way exceeded the measured value, then the measured value was set as the maximum possible value (i.e., it was assumed that MPP contributed 100% of the measured particulate sulfate concentration).

Key assumptions of the Tracer Scaling method applied to particulate sulfate attribution includes the following: (1) The tracer and sulfur (emitted as SO_2) are transported and dispersed identically together to the receptor; (2) There is no deposition of tracer or either SO_2 or particulate sulfur enroute (or they all deposit at the same rate); and (3) The tracer/SO_2 emission ratio is constant (i.e., the PFT emissions rate tracked the variations in the SO_2 emissions rate). In actuality, SO_2 and sulfate will undergo some deposition in route, while the tracer is essentially non-depositing; therefore the ratio of sulfur to PFT decreases in time. The assumption of a constant ratio will only be true for extended periods of near constant SO_2 emission rate since the tracer emission rates were held constant (except for the timing tracers).

The fundamental assumption of the Tracer Scaling approach applied to particulate sulfate is that all of the SO_2 is assumed to convert to particulate sulfate or at least enough of it is converted to match the sulfate concentration measured at the receptor. This assumption produces an upper-bound impact of the tracer-tagged source -- it is impossible to have a higher contribution. A lower contribution is certainly possible and is likely, especially in the cloud-free conditions under which sulfate formation proceeds slowly. Application of Tracer Scaling to primary pollutants is expected to produce an upper bound value that is likely to be much closer to the true contribution.
The principal benefit of tracer scaling is to place a firm upper limit on attributed pollutants from tagged sources that can be used to identify periods when other methods must be incorrect. It needs to be re-emphasized, however, that the Tracer Scaling estimates of secondary particulate species do not indicate what a realistic contribution might be.

For BRAVO, the direct use of tracer scaling for the Carbon I/II plants will not be possible due to the use of a surrogate site at Eagle Pass to approximate a Carbon release. For the stack releases of PFT, the tracer scaling approach could be used directly, but is not expected to be particularly useful in this regard because only 2 of many eastern Texas power plants will be tagged directly. The primary use for these releases is to quantify transport and dispersion properties of the airflow that may be expected to similarly affect other elevated pollution sources.

RMAPS

A spatial pattern correlation receptor model, RMAPS (Henry, 1997a) was used in Project MOHAVE to apportion the average concentration of a species, as measured at many sites, among several spatially distinct sources. It can be applied to primary or secondary species; no assumptions concerning transformation or deposition rates are required.

RMAPS was applied to predict the impacts of emissions from several source regions, including one identified as the "Colorado Valley Source" located in the vicinity of MPP and the Las Vegas area (Henry, 1997b). Green and Tombach (2000) describe tests of the RMAPS concentration predictions for the Colorado Valley Source against the maximum particulate sulfur that could be attributed to MPP based on measured PFT concentrations and assuming 100% conversion of SO_2 (Tracer Scaling). This comparison was done at 21 receptor locations, with concentrations averaged over the summer intensive.

The RMAPS-predicted spatial patterns for emissions from the Colorado Valley Source showed significant impact south of MPP, while such impact was not observed in the tracer data. Specifically, for 13 of these receptors, mostly located in the 180-degree sector to the south of MPP, the RMAPS predictions exceeded the maximum amount of particulate sulfur that could be created from MPP emissions. The excess was sometimes more than a factor of two and in all cases was well beyond the uncertainty bounds assigned to the RMAPS and PFT tracer calculations. Based on these observations, Green and Tombach (2000) concluded that the RMAPS predictions of the impacts of the Colorado Valley Source are not a valid representation of the impacts of MPP. The reasons for this discrepancy were never determined.

RMAPS will be applied to the BRAVO Study data in an attempt to identify significant source regions and their contributions to Big Bend aerosol concentrations. As in Project MOHAVE, its results can be checked against other methods including Tracer Scaling.

Tracer Regression.

Another simple method employed in Project MOHAVE involves use of multiple linear regression analysis to explain the variations in light extinction data at the primary receptor site by the variations in the concentrations of several source-specific tracers. In that study the tracer regression method (White *et al.*, 1999) attempted to explain light extinction at Meadview based on contributions from three sources – MPP, Southern California, and southern Arizona/northern Mexico. The light extinction was related to these source contributions through multiple linear regression analysis, in which assumed markers for each of the three sources were the independent variables and b_{ext} at Meadview was the dependent variable. Methylchloroform (an industrial solvent) was taken to represent urbanized Southern California, the mixing ratio of water vapor to air was taken to represent the contribution of air from more humid regions to the south, and the PFT to represented MPP emissions. In each case, the tracer was assumed to be a conservative indicator, as required by the receptor-oriented regression procedure.

The principal assumptions of the tracer regression method have to do with source types or regions represented by each tracer. Except for the use of PFT for tracer-tagged sources, these assumptions involve approximation. Endemic tracers for the BRAVO Study are yet to be identified and as in Project MOHAVE it is unlikely that possible other sources of those materials can be completely ruled out. If the tracers are not unique to the

region or source to which it is assigned, then emissions will be attributed erroneously to that region or source.

It should also be noted that any regression analysis of this kind would underestimate attribution if the "signal" were noisy, as would be the case if the light extinction were to vary because of unaccounted for background effects. (This limitation also applies to other regression based methods such as TMBR below).

TMBR

Tracer Mass Balance Regression (Malm *et al*., 1989; Ames and Malm, 1999) was used in Project MOHAVE to compare the covariance of SO_2 or particulate sulfur measurements with those of the PFT through an ordinary least-squares regression. The regression coefficients were interpreted as indicators of the attribution of the sulfur constituent to MPP.

While TMBR produced a significant regression coefficient (P=.03) in Project MOHAVE which means that there was a highly significant statistical relationship between PFT concentration and ambient sulfate concentration at Meadview, only a small fraction of the ambient SO_4 variability was explained by PFT ($r^2 = 0.06$). This may result from the non-linearity of secondary sulfate production and so these TMBR results alone could not be used to quantify any level of contribution by MPP.

TMBR applications in the BRAVO Study are limited to tracer-tagged sources but can be applied to any emitted pollutant.

DMBR

Differential Mass Balance Regression (Latimer *et al*., 1989, Ames and Malm, 1999) applied to Project MOHAVE expanded on the TMBR approach by explicitly considering the conversion of SO_2 to particulate sulfur. In this hybrid approach, information about transport time from source to receptor and cloud cover was used with linear conversion and deposition rates to estimate the particulate sulfur concentration at the receptor. The rate constants for the conversion of SO_2 and for SO_2 deposition were chosen by statistical optimization of the correlation between the predicted MPP contribution to SO_2 at Meadview and the measured SO_2. This optimization procedure made no *a priori* assumption about the amount of variability explained by the MPP contribution to ambient SO_2.

In addition to the usual constraint on equivalent behavior of tracer and sulfur emissions, the DMBR method estimated the amount of conversion of SO_2 to particulate sulfur based on a linear conversion rate. The time of travel was estimated from a wind field model and an hourly conversion rate was derived empirically based on a Cloud Interaction Potential (CIP) and the measured concentrations of SO_2. The CIP, derived from observations of clouds in photographs, attempted to reflect the presence of cloud water in the conversion process. But, since the height of the clouds could not be readily

deduced from the photographs, the CIP was considered a crude indicator of the effect of cloud water on chemical reactions at the MPP plume height.

As with TMBR, application of DMBR in the BRAVO Study will be limited to attribution estimates of tracer-tagged sources.

TAGIT

In Project MOHAVE the Tracer-Aerosol Gradient Interpretive Technique (TAGIT) (Kuhns *et al.*, 1999) used PFT data to identify sites near a receptor site that were not significantly impacted by MPP during specific sampling periods and could be considered to represent the regional background concentration. The MPP-attributable particulate sulfur at a receptor was calculated as the measured excess concentration of sulfur over that at nearby sites with background levels of tracer. Sites with tracer levels below 3 sigma of the background concentration were considered to be representative of regional background sulfur concentrations.

The accuracy of TAGIT depends on the assumption that the only cause for increased sulfur above the regional background at locations where PFT is found was emissions from MPP. If sulfur from another source were transported along the same trajectory as that of MPP, then the assumption would be violated. Under those conditions TAGIT would have erroneously apportioned to MPP the sulfur from the non-MPP source. Because the difference in sulfur particle concentrations in PFT impacted and non-impacted areas was sometimes small, TAGIT occasionally attributed a small negative concentration impact to MPP. The precision of the TAGIT attribution was estimated when there are several nearby sites reporting background tracer concentrations near the impacted receptor. For many instances, the variability of these multiple estimates were larger than the particulate sulfur attributed to MPP by TAGIT. While individual attibutions by TAGIT were noisy, the method was thought to provide credible results of average attribution over the study period.

Application of TAGIT in the BRAVO Study was anticipated in the study design with the location, near Big Bend, and higher time resolution of the 6-hour monitoring sites. These should give a much-improved ability to determine background near Big Bend, which should enhance the performance of TAGIT for sulfate and SO_2. While conceptually TAGIT can be applied to any pollutant, the short time periods and use of only the IMPROVE sampler channel A ($PM_{2.5}$ mass, PIXE and XRF) at the 6-hour sites is expected to restrict the assessment principally to SO_2 and particulate sulfate attribution.

The high time resolution sulfate, SO_2 and tracer data at Big Bend will be used to apply a variant of TAGIT that would operate in a temporal instead of a spatial sense. This temporal TAGIT would use periods before and after a tracer hit at Big Bend as the background concentrations to be subtracted from the concentrations measured during the tracer hit.

As the release of PFT from the Carbon I/II stacks was not possible, use of the Eagle Pass releases for TAGIT may or may not be fruitful. If ambient data show high

correlations between SO_2 and Eagle Pass released PFT at nearby sites, this would argue for the use of Eagle Pass releases as a surrogate for Carbon I/II emissions. The possibility of emissions from the tracer tagged stacks at Big Brown and Parish power plants with other SO_2 sources limits the applicability of TAGIT to these sources.

CMB

The Chemical Mass Balance technique involves apportionment of the composition of the aerosol at receptors among "profiles" of the composition of emissions from various classes of sources. The product of the analysis is an apportionment of the pollutants that are assumed to be conserved including primary particulate species and SO_x (the sum of SO_2 and particulate sulfate) to the selected classes of sources.

CMB assumes that time-invariant source profiles are available for all of the sources or source types to be attributed and that these are conserved during transport from the source to the receptor location. Both of these assumptions are most realistic for sources of primary pollutants that are near the receptor location. For this reason CMB has proven to work well in urban settings to explain local impacts of well-characterized primary pollutant sources. The success of CMB for a remote receptor location where attribution of distant sources is desired is more problematic. In such situations, the number of possible source that may be influential is potentially large so that during any sampling period a large number of sources may be contributing each with a relatively small impact, and sources profiles may change in the atmospheric (deposition & conversion) during long-distance transport.

One CMB type of approach that was tried during Project MOHAVE to account for the potential change in source profiles during transport is to use an effective source profile based upon ambient monitoring data during a period of assumed direct impact from various sources areas. The method (Eatough, *et. al.,* 1999) was employed by investigators to attribute SO_x and particulate sulfate. The Modified CMB (MCMB) method used several elemental and chemical tracers of opportunity as marker species for MPP and major source regions (the Las Vegas area, urban Southern California, the San Joaquin Valley, Baja California, southern Arizona and northern Mexico). The source profile for each source region was determined by measuring the elemental and chemical composition of ambient aerosol approaching the study area from the direction of the source of interest. The chemical conversion of SO_2 to sulfate was addressed using reactivities derived from the Reactive and Optics Model of Emissions (ROME) (a Lagrangian model for particle formation in plumes) and from optimization of assumed linear conversion rates. The transport routes and times of travel were defined by several wind field models and the potential for clouds to affect the chemistry during the transport of MPP emissions was addressed through the Cloud Interaction Potential (CIP) of the DMBR model. It is important to note that the PFT concentration data were used in the evaluation and modification of the model, but are not used as input data.

Fundamental assumptions of the MCMB method were the equal conservation of the tracer and target species and that all significant contributors to SO_2 and sulfate at

Meadview and Hopi Point were identified in the CMB profiles. A further assumption in the MCMB approach was that the ratio of SO_x (sum of SO_2 and sulfate) to the marker species in the source profiles is constant from day to day. Profiles and the profile uncertainty for regional sources, such as Southern California, were developed from ambient measurements at substantial downwind distances during a few days. If the ratios varied outside the determined uncertainty or represent mixes of materials from different source regions the method would apportion SO_2 and sulfate incorrectly among sources. Furthermore, regional profiles tended to be more collinear and less orthogonal than profiles for discrete source types.

A fundamental conceptual problem with use of ambient data as source profiles is the circular reasoning that comes from the use of ambient samples for periods thought to be principally influenced by a specific regional source as the source profiles. These source-specific sample periods were selected by using crude trajectory analysis, making the results subject to all of the uncertainties of the trajectory analysis. MCMB is not scheduled to be used in the BRAVO Study but is described here to illustrate the variations of the CMB that have been used in previous studies and could be developed for use with BRAVO data. Standard CMB analysis will be applied using the source profile information collected for the BRAVO Study. It will also be used to attempt to apportion the particulate organic material using speciated organic source profiles and ambient samples for selected time periods.

Artificial Neural Networks

Neural networks can be used in receptor modeling where source profiles are not known. The self-organizing ANN method of Kohonen (1989) has been presented for local scale problems with a single sampling site (Wienke and Hopke, 1994 a&b) and for multiple sampling sites (Wienke et al., 1994). This method can analyze a three dimensional data bloc as a whole and yield both source profiles and geographical information on the identified emission sources. Application of this type of sophisticated assessment to the BRAVO Study offers a way to compare source profiles as measured at the source with estimates of the effective source profiles at the receptor locations.

Trajectory – Back-trajectory Analysis

Trajectory and back-trajectory analysis methods are based upon calculated transport paths of air parcels. Surface and/or upper level wind measurements are either interpolated or used as input to a meteorological model to create a series of wind field (i.e. two or three dimensional maps of wind speeds and direction) as a function of time. Trajectories are calculated by moving the air parcel from a user selected starting point at a specific time in the direction and at the speed of the wind as determined by the appropriate wind field. With each time step the air parcel is again moved based upon the wind speed and direction at the new point and time to generate the trajectory path. Back-trajectories are calculated in the same way except that the time steps are run back in time and the path generated shows where the air parcel that arrived at a user specified time and location is thought to have taken on its way there. The HYSPLIT trajectory model run

using the Eta Data Assimilation System (EDAS) output will be used in the BRAVO Study as the principal trajectory analysis method. EDAS assimilates observed data into short-term Eta model calculations to obtain meteorological fields. Example HYSPLIT back-trajectories from Big Bend National Park are shown in Figure 5-5.

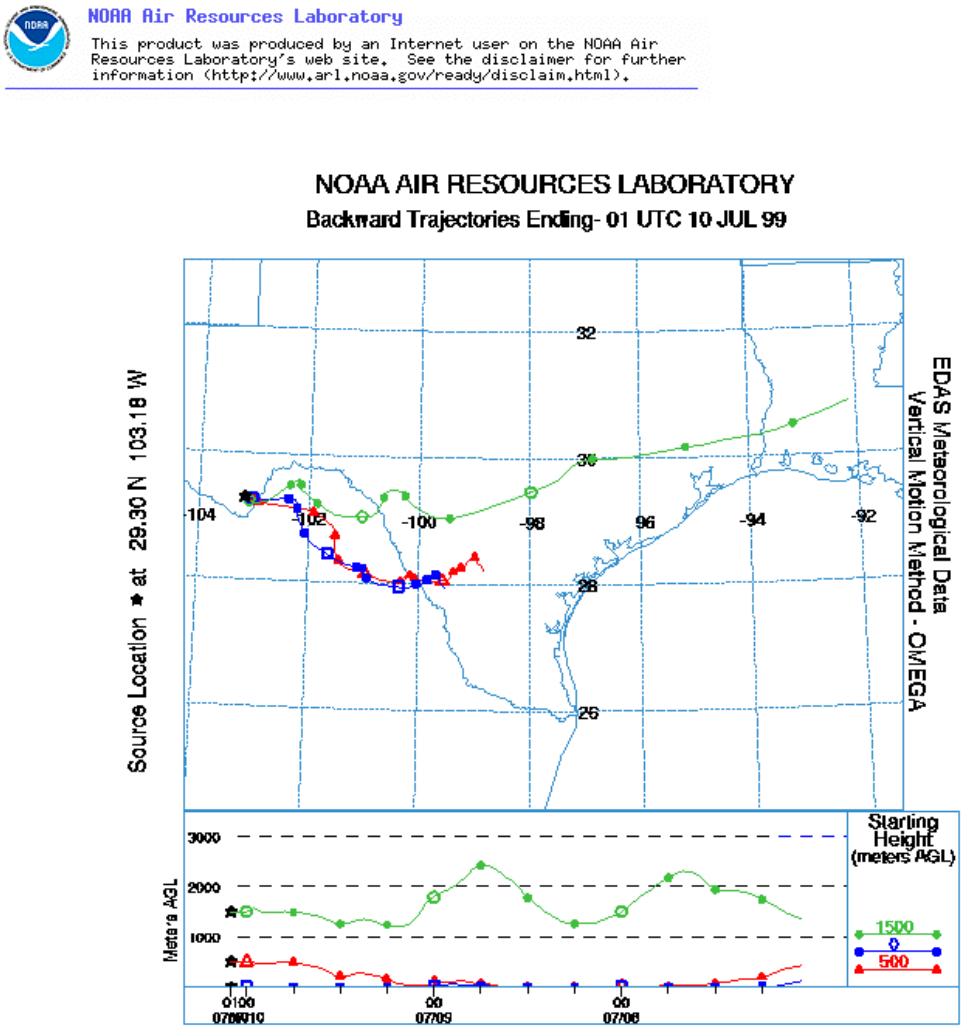


Figure 5-5. Example HYSPLIT back-trajectories from Big Bend National Park for July 10, 1999. The back-trajectories were started from 0, 500 meters, and 1500 meters AGL and were run backward for 72 hours. Differences in trajectories between the near surface and 1500 m level reflect some wind shear with height. The map view shows the horizontal path of the back-trajectory, while the time series plot shows the vertical path as a function of time.

NOAA-ARL will create an archive of EDAS output at 40 Km grid spacing for the BRAVO study period (July 1- October 31, 1999) for use in HYSPLIT. This will provide for archival of data at all grid points, rather than at every other grid point currently archived for HYSPLIT use. BRAVO participants will be provided access to a fully functional version of HYSPLIT that can be used to run forward and backward trajectories for periods of 5 days from any user selected location within the EDAS domain. Output will include graphics showing trajectory pathways, concentration isopleths, etc. and

trajectory endpoint files. Users will be able to run "batch modes"; this would include running trajectories for many time periods and running trajectories/dispersion forward from multiple sources.

After the BRAVO study period concludes (October 31, 1999) a copy of the archived EDAS data sets and HYSPLIT model will be submitted to the BRAVO database manager (DRI-Las Vegas) on CD-ROM. The CD-ROM will include the necessary structure so that HYSPLIT may be easily run from the CD-ROM. The BRAVO database manager will distribute copies of the CD-ROM to BRAVO participants upon request.

Trajectory analysis assumes that the calculated wind fields are good representations of the true wind fields and that a single point can represent the air mass location at any point in time. The first of these involves both measurement uncertainty and the capabilities of the method used to generate the wind field from those measurements. Errors in calculated air parcel position that are associated with imperfect wind fields tend to increase with each time step. Trajectory-calculated air parcel positions more than just a few days (i.e. 3 to 5) from the initial location are generally thought to be uncertain by hundreds of kilometers. Position errors can also be substantial for short-duration trajectories under rapidly changing meteorological conditions such as frontal passage.

The concept of an air parcel used in trajectory analysis is rather vague, but for any practical use it must have some non-zero dimension that can be thought of as containing the emissions of a specific source or sources in a specific area (e.g. a city) for some short period of time (minutes to hours). A point at the center of mass of the air parcel can be used to represent its location at the point of origin. However, the integrity of an air parcel is typically very short-lived because of the effects of turbulence and wind shear. These will cause the air parcel to spread out (e.g., vertically in the mixed layer on a hot summer day) and can cause it to divide into disjointed pieces (e.g., part of the air parcel can be sheared off and separated from the rest). Even if the trajectory path could be perfectly calculated, it may be very misleading to think of its position after several days of transport as of the center of the air parcel distribution.

In spite of the uncertainties, trajectory and back-trajectory analysis have a number of important uses in attribution analysis all of which will be used in the BRAVO Study. Since trajectory methods don't calculate dispersion and deposition they cannot be used directly to determine source contributions at a receptor site. However, they can be used to identify time periods where emissions from specific sources are thought not to contribute at a receptor site because the transport was in a completely different direction. In this way trajectories can be used as an independent check of the reasonableness of receptor modeling attribution results (i.e., check whether the trajectory path connects the receptor site with the primary contributing sources identified for each sample period). Some receptor methods use trajectory analysis-predicted emission age (i.e. transport duration from emission to the receptor locations) to estimate sulfate concentration from a specific source using typical SO_2 to sulfate conversion rates. Comparison of trajectories calculated using wind fields determined by different methods is a simple method to

determine whether the wind fields are significantly different with regard to transport. Trajectories from tracer-tagged sources can be compared to the PFT ambient concentrations at the monitoring sites to evaluate the combined accuracy of the wind field and trajectory algorithm. Statistical associations may be developed between the amount of time air parcels are estimated by trajectory analysis to spend over various source areas and the corresponding receptor site air quality level (e.g. sulfate concentration, light scattering coefficient, etc). Typically this has been done with back-trajectories for sites with multiple years of ambient monitoring data, but it will be tried with some of the sophisticated measurements made during the four months of the BRAVO Study.

CALMET/CALPUFF

CALMET/CALPUFF is a combination of a diagnostic meteorological model (CALMET) and a Lagrangian puff air quality model (CALPUFF) that was used in Project MOHAVE to predict Mohave Power Project (MPP) impacts. Hourly radar profiler wind data was used as input data for CALMET. The choice of input wind data and how to set up the model to use it were made to increase the ability of the model to predict the ambient PFT data. The grid scale of the wind field was 5 km, which was sufficient to represent major topographic features but smoothed over many smaller ridges, peaks, and valleys. The Pasquill-Gifford-Turner (PGT) diffusion algorithm, with transitioning to time-dependent dispersion curves at longer distances, was used to represent the plume diffusion. CALPUFF simulates daytime SO_2 conversion to particulate sulfur using a linear mechanism with a conversion rate that is based on solar radiation, PGT class, ambient ozone concentration, and relative humidity. The algorithm produces a maximum conversion rate of about 4%/hr at 100% RH, which is lower than generally-accepted peak aqueous conversion rates. On the other hand, the algorithm does not attempt to quantify the time spent in clouds, which could produce a lower hourly-average rate than the peak that occurs whenever the plume is in a cloud.

In Project MOHAVE the CALPUFF/CALMET system was used to simulate two types of conditions, both of which may be considered as bounds to the range in which actual impacts of MPP might lie. One type of conditions was based on the assumption that all sulfate formation took place in cloud-free air. This can be considered to produce a lower bound with respect to actual sulfate formation. The other type of conditions that was simulated was based on the assumption that the MPP plume interacted with clouds for a specified period of time each day. Because clouds were not present every day and the assumed period of interaction was long compared to conversion rates in clouds, this condition was taken to approximate an upper bound to potential source impacts.

For the first type of conditions, the internal chemistry algorithm of the model was used to calculate the conversion of SO_2 to sulfate. This algorithm is based on homogeneous, “dry” chemistry. For the second type of conditions, where the MPP plume was assumed to interact with clouds, aqueous phase chemistry was likely to occur, which would result in much higher conversion rates than the internal algorithm of the model would predict. Therefore, as a bounding exercise, for the second analysis it was assumed that all the plume material interacted with clouds for three hours every day and the SO_2 was converted to particulate sulfate at a rate of 20% per hour during those three hours.

These two analyses, labeled "CALPUFF Dry" and "CALPUFF Wet," respectively, can be considered as estimates of lower and upper bounds to the impacts of MPP emissions The initial settings and choices of input meteorological data were selected to improve comparisons between predicted and measured PFT concentrations (Vimont, 1997).

All air quality simulation models are subject to uncertainties associated with the limitations of spatial and temporal resolution resulting from practical computational restrictions, input data uncertainty and/or lack of representativeness (e.g. meteorology, air quality, & emission data), and assumptions and parameterizations to required to provide the myriad input information not available from measurements. Even in models that incorporate terrain, it is typically done so by accounting for the average terrain elevation of a rectangular grid at the surface which is often much larger than critical terrain dimensions. Canyons, narrow mountain passes and ridges that may be influential to flow and dispersion are not well characterized by the model-generated virtual terrain of uneven height cell-sized blocks. Uncertain or non-representative measurements used as input to air quality models result in some level of prediction uncertainty depending on the model's use of the data. Model sensitivity analysis is a standard approach to evaluate this source of uncertainty. Sensitivity analysis can also be used to evaluate assumptions and parameterizations but it is rarely done on more than a small fraction of the many assumptions because of the effort involved.

In the BRAVO Study CALPUFF will be used as a tool to evaluate the utility of various input data, wind-fields, etc. by identifying those that yield the best comparison between predicted and measured PFT concentrations. Presuming it produces credible results; CALPUFF will also be available as a sort of general-purpose regional air quality model that can be used to perform reality checks on results of receptor source apportionment methods. As in MOHAVE, it will also be used to estimate sulfate impact bounds for some of the major SO_2 point sources to provide a possible range of impacts that corresponds to whether or not cloud chemistry occurs.

Lagrangian models like CALPUFF are most appropriate to simulate one or a few isolated emission sources that are relatively near to the receptor location (e.g. Carbon I & II with respect to Big Bend). However, they are limited in that they treat each source's emissions separately and combine the results, so that chemical interactions of pollutants from different sources cannot be simulated. They also tend to be awkward to use if emissions from many sources are to be combined. With this in mind CALPUFF will not be depended upon to simulate all major sources in the study region that contribute to Big Bend haze.

REMSAD

The Regulatory Modeling System for Aerosols and Deposition (REMSAD) modeling system was designed to estimate particulate concentrations averaged over horizontal grid scales of roughly 20 km and with a vertical resolution of 50 to a few hundred meters. It is capable of treating sub-domains at higher resolution, which allows savings of computer time in outlying areas of lesser interest while still resolving the areas

of greatest importance (e.g. receptor locations). The particulate concentrations can be broken down into size categories (and mass distributions) and the predictions can include the effects of photochemistry.

The REMSAD core model for aerosol and toxic deposition (ATDM) is a three-dimensional grid (Eulerian) model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. The pseudo-first order PM oxidation chemistry package from RTM-II has been incorporated, and the dry and wet deposition routines have been updated to include additional species.

The model framework extends vertically to treat the entire troposphere with a sigma (terrain following) vertical coordinate. It can provide two-way interactive nesting of fine grids within coarser mesh grids in both the horizontal and vertical. The model uses a precomputed hydroxyl chemistry package based on a multidimensional lookup table. This table takes into account variations in pressure, temperature, moisture, solar intensity, clouds, ozone, NO_x and a representative VOC species. The model includes a cumulus convective parameterization scheme and a stratiform parameterization scheme for the distribution and removal of pollutant species.

In addition to the fundamental assumption that are required for any air quality simulation model (indicated above for CALPUFF), Eulerian air quality model such as REMSAD are subject to numerical dispersion. Input and predicted conditions are assumed to be uniform in any grid cell. If a receptor location is within one or two cell dimensions of a source being monitored, a Eulerian model will indicate a greater than true frequency of impacts that are of lower than true concentrations. This happens because the true plume is much narrower than the cell it is in causing it to miss the site more than in the simulation, and it is more concentrated than the cell-averaged concentration in the simulation.

The primary purpose of REMSAD for the BRAVO Study is to estimate haze impacts at Big Bend of all the major emission sources in the region. It is the only method proposed for use in the BRAVO Study that has the capabilities to estimate impact for all sources in the region for which there are emission rate data. Other methods are limited to certain pollutants, to artificial tracer-tagged sources, sources for which there is a prominent endemic tracer or to large sources near Big Bend. This is not to say that REMSAD results will be accepted without critical evaluation. In fact the very purpose of employing multiple attribution methods is to permit comparisons and evaluations (further discussed below in the section on Reconciliation of Results). REMSAD use in BRAVO may be modified to mitigate problems identified during the reconciliation process and improve performance. Also the level of uncertainty ascribed to its results may be modified to reflect its performance compared to other methods.

Table 5- 3 shows the responsible organization, the sources that can be examined and the particulate species and/or optical parameters that will be addressed for each of the attribution methods discussed above.

Attribution Method	Responsible Organization	Attributable Sources	Attributed Components
Tracer Scaling	DRI	PFT-tagged	Sulfate, SO_2, primary particles
RMAPS	NPS	All source by areas	All major PM species
Tracer Regression	DRI, NPS, & TNRCC	PFT & endemic-tagged	Light extinction, all major PM species
DMBR	NPS	PFT-tagged	Sulfate
TAGIT	DRI	PFT-tagged	Sulfate, SO_2, primary particles
CMB	NPS, DRI, & CSU	All sources with profiles	Primary PM species, SO_x, organic species
Neural Networks	NPS (Phil Hopke)	All major sources	Primary PM species, SO_x
Trajectory	NPS, DRI, & TNRCC	All major sources	Light extinction, all major PM species
CALPUFF/CALMET	NPS	Selected major sources	All major PM species
REMSAD	NPS	All large sources	All major PM species

Case Studies and Episode Analysis

Analysts preparing case studies and conducting episode analysis draw on diverse measurement data and model results to construct a story (or conceptual model) that explains how sources produce impacts and why the pollution levels at monitoring site change over time. Case studies usually focus on what is happening with emissions from a source (or sources) and in that way are analogous to air quality simulation models, while episode analysis tends to focus on why the pollutant concentrations or haze level is changing at a receptor location which is analogous to receptor modeling. Both are documented by the preparation of descriptive narratives that illustrates our understanding of the phenomenon of importance. Case study and episode analysis is performed because none of the attribution methods provides this type of a direct and clear answer to questions such as these: How does that source's emissions cause haze? How do atmospheric processes contribute or reduce the impacts of responsible sources? What is the sequence of events that leads to the changing impacts at the receptor location?

In addition to addressing these types of questions, data analysts performing case study and episode analysis typically draw on a variety of information, some of which may not have been explicitly used in any of the attribution methods. This provides valuable opportunities to further challenge conceptual models and the results of attribution methods by comparisons with independent information. If these challenges result in consistency, the conceptual model gains credibility; if the result is inconsistency, either the model or the independent information it is being compared with must be incorrect.

One of the most important uses of case studies and episode analysis is to communicate with non-technical interested people (e.g. the public, policy makers, etc.)

concerning our understanding of the important processes responsible for haze at Big Bend. Generally it is not enough to summarize the results of an attribution study in tables and graphs, interested non-experts want an explanation of how emissions from various sources and the atmosphere work to generate these results. Without such explanations, the results may not be fully believed and/or inappropriate public policy may be promoted to deal with a misconceived understanding of the situation (e.g. control of a source that is a substantial contributor thinking that it will improve summer haze episodes, but the source rarely contributes in summer).

Air quality modelers and receptor modeling data analysts usually do some level of case study and episode analysis as a means to communicate and sell their methods' results. These will be compared and expanded on by DRI scientists to compile a set of descriptions of case studies and episodes that are self-consistent and in accord with independent information.

Computer Simulation of Visual Air Quality

In order to assist in interpreting the quantitative data of impacts on the light extinction coefficient, b_{ext}, various levels of visibility degradation in typical Big Bend National Park views will be displayed in images that can be viewed on a computer screen. Mathematical models of radiative transfer will be used to calculate the changes in the appearances of these views due to various levels of light extinction. The approach used to generate these simulated views is described here.

Radiant energy, as it passes through the atmosphere, is altered by the scattering and absorption by gases and particles. Image-forming information is lost by scattering of radiant energy out of the sight path and absorption within the sight path. Further, ambient light from direct, diffuse, and reflected radiance is scattered into the sight path. This adds radiant energy called "path radiance" to the observed radiation field.

The transmittance of the sight path is calculated from measured extinction or the distribution of particles and gases along the sight path. The path radiance is more difficult to estimate. A reasonable assumption under uniform illumination (cloud free sky or uniform overcast) is to estimate the path radiance with an equilibrium radiance model.

Equations for path radiance and observed image radiance are applied to each pixel of a photographic image, to represent the effect of the atmosphere on that image. The bulk atmospheric optical properties such as extinction, scattering, and absorption coefficients, single scattering albedo, and the scattering phase matrix are required to apply the equations to each element of a scenic view. They are calculated by an aerosol model. The Mie theory model assumes spherical particles for externally-mixed, homogeneous or internally-mixed, coated aerosols.

A backward photon trajectory, multiple scattering, Monte Carlo, radiation-transfer model will be used to calculate sky radiances. The inherent radiance of each terrain pixel

will be estimated with the equilibrium radiance model, sky radiance model, and distance to the target for each pixel.

The modeled image radiance field for a selected level of extinction will then be calculated by first using the new extinction value and distance to each terrain pixel to calculate a new path transmittance. Second, the new path radiance will be calculated using this transmittance and modeled sky radiance. Third, the new apparent image radiance field will be calculated. These new image radiance files will then be used in the image processing modules to generate the final images, as described below.

The original images that start the process described above will be 35 mm color slides taken at Big Bend National Park. The slides necessarily will represent cloudless skies under the cleanest visual air quality conditions possible. Aerosol and optical data associated with the day the picture was taken will also be used. The slide images will be digitized through three wide band filters at different colors.

To produce the new image, which displays the scene appearance at a chosen level of extinction, the new radiance field is calculated as previously described. That modeled radiance field describes the appearance of every pixel on the photograph, each of which has been altered by the scattering and absorption that were artificially added to the initial image. The results, when viewed as a photograph or on a color computer monitor, then portray the original digitized photograph under the different atmospheric conditions.

The simulation of human perception of actual scenes by using photographs or computer images is not perfect. Based on color matching experiments performed at the Grand Canyon, Henry (1999) points out that such images are less colorful and more blue than the true scenic view that is observed on site. These conditions appear to derive from the limitations of the photographic film that is the basis for the initial images that were digitized. A consequence of these limitations is that the artificial images overstate the visual effects of increasing haziness.

Consequently, one should not rely on the computer images to provide quantification of thresholds of human perception of visibility change in terms of extinction changes. Rather, these images should be considered approximations that portray the essential effects of extinction change, albeit only semi-quantitatively.

5.6 Reconciliation of Results

Reconciliation of results is a process that begins in an informal way midway through the data analysis phase of the study, but can only be completed near the end of that phase. Each of the attribution assessment approaches produces results that address the contributions by emission sources to visibility impairment measured at Big Bend. Preliminary results of these methods will be shared internally among the study participants (other analysts, sponsors, etc.) at data analysis meetings as results become available. This process of technical communications is expected to spawn critical review,

comparisons with other methods, and method refinements. There may be several rounds of review, refinement and reapplication for some methods. Initially only about half of the PFT measurement data will be distributed to the data analysts to use in any way they choose in their models (i.e. input data or to refine the methods), but towards the end of the data analysis phase of the study the rest of the PFT data will be released and used to evaluate the methods. This may provide valuable insight concerning which models are credible and may convince some data analysts to withdraw their method as unsatisfactory for BRAVO. Shortly after the release of the last of the PFT data, final results from the surviving methods will be compiled. There is no expectation that the results of the various methods will be consistent with each other at that point in the process.

At this point in the process, it is necessary to reconcile what may be disparate final results in order to produce the BRAVO Study findings. Reconciliation involves judgments of the credibility of technical information. These are based principally on a process of inter-comparing information from independent sources. Some technical information is inherently more credible than other information. An information credibility hierarchy can be constructed which divides sources of information in to three groups based upon its source. The most credible source of information is generated directly from well-established physical principles and involves few if any assumptions. Examples include: pollutant concentrations must be positive, and pollutants are transported in the direction of airflow. The next category of information sources contains well-characterized measurements and simple parameters derived from them. These are assumed to be credible within their uncertainty bounds. The category of information with the least credible information includes results from physical and statistical models, which contain the combined uncertainty of input measurements and model assumptions.

The most productive comparisons are between model results and measurements or physical principles. An inconsistency with information from these more credible sources is a strong indication that the model result is not correct. However a consistent comparison does not ensure that the result is correct, and there may be situations where the comparison is indeterminate or no comparison can be made. It is also likely that models may work satisfactorily for some situations but be unsatisfactory for other situations. So a poor comparison for some of the periods does not necessarily mean the model results should all be ruled unreliable.

In spite of the relatively poor power to resolve credibility issues between information sources in the same category, a systematic intercomparison of results from all of the attribution models will be conducted. This is made more difficult because many of the attribution models address sources in quite different ways (e.g. specific sources, source areas, source types). The predictions of each of the attribution model for every sample period at the primary receptor site will be compared. The next steps depend on the results of these comparisons. If there is substantial agreement among many of the methods most of the time, then the outlier methods and time periods will be examined to attempt to understand why they seemed to disagree. It is also important to determine whether the methods that agreed do so because they are not very independent (i.e. use the same input data in much the same way) in which case their agreement does not greatly

increase the credibility of their results. Alternatively, if very independent methods produce results that substantially agree, their results do gain in credibility.

If the model results do not group or if the methods that do seem to group are all interdependent then there may be no basis for deciding which is more credible for any particular sample period. This was the situation in Project MOHAVE, where the results that agreed best on a daily basis all depended on measured PFT concentrations. An irresolvable inconsistency on a sample period by sample period basis represents a serious degradation of study finding credibility, but it does not necessarily mean that the study is without useful results. In the Project MOHAVE case, the primary question was the impacts of MPP at the primary receptor site. While the methods did not agree on which days had the biggest impacts, they did define a rather narrow range of impacts for the worst days that each identified. Cumulative frequency distribution plots that showed the range and frequency of impacts by each method for the period of the study illustrated this, which was a useful finding of the study. Figure 5-6 shows the cumulative frequency distribution of 12-hour sulfate attributed to MPP by various models and bounding calculations.

In addition to determining credible attribution results, the reconciliation process will determine suitable uncertainty limits to associate with those finding. In Project MOHAVE it was the range of results at any frequency (e.g. 50^{th} percentile or 90^{th} percentile) from the various attribution methods.

The BRAVO Study Technical Manager working with DRI and in close consultation with the technical steering committee will be responsible for the overall reconciliation of the study attribution results.

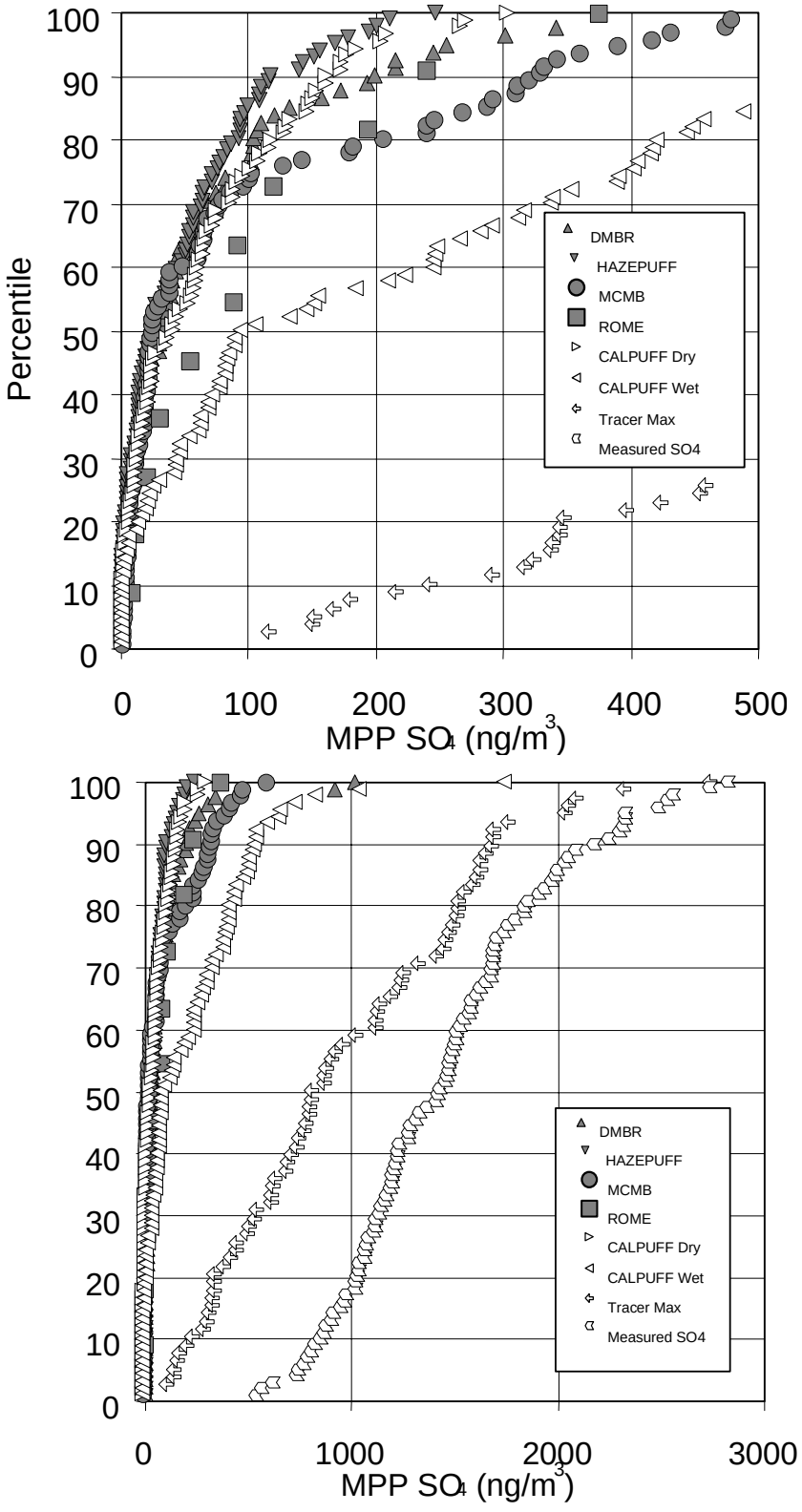


Figure 5-6. Cumulative frequency plots of 12 hour sulfate attribution to MPP at Meadview during the summer intensive. Note: filled symbols represent estimates of MPP attribution; open symbols indicate bounding calculations and physical upper bounds.