11. Attribution

Overview

The attribution analysis will be done using a variety of analytical tools; particularly deterministic, hybrid, and receptor models; and the MPP emission modulation study. Deterministic modeling is an approach that attempts to explicitly account for physical and chemical processes transporting and acting on emissions from a source. Receptor models use measurements made at the area of concern (receptors) along with characterization of the emissions from sources potentially affecting the receptors. The contribution of each source to concentrations at the receptors is determined statistically through multivariate analysis techniques which link the sources to the measured concentrations. Hybrid models use a combination of deterministic and receptor modeling techniques. Apportionment implies determining the concentration of sulfate at the receptor areas resulting from MPP and other sources. The apportionment of secondary aerosols such as sulfate is a complex problem as noted by the National Research Council (1990) and others. Transport, dispersion, deposition, and transformation must be accounted for.

Results from the extinction budget analysis will be used in conjunction with the sulfate attribution to determine the fractional contribution of MPP sulfate to the extinction coefficient. The effect of primary particles will also be considered. The next step is to evaluate the perceptibility of the contribution of MPP to the extinction coefficient. Finally, the question of the effect of reducing emissions from MPP upon visibility will be addressed. Each of the main study components used in the attribution analysis is described in the following sub-sections.

The results from the various models and analyses will be compared and reconciled. Reconciliation is a critical component of the analysis. If results from a particular model or analysis cannot be reconciled with other analyses, the results will not be used. The range of uncertainty in each calculation and the reconciled results or consensus will be estimated.

A major area of concern that has been expressed by some is the possibility for misuse of tracer data for source apportionment. Specifically, two issues have been expressed: (1) that any tracer level above background measured at the receptor sites will be interpreted as attribution of visibility impairment by tracer sources; (2) that tracer data will be incorporated into analyses inappropriately by repeated regression analysis with whatever parameters and formulisms are needed until a statistically significant relationship is found, though no physical relationship is evident.

Project MOHAVE planners <u>do</u> <u>not</u> interpret the appearance of any tracer above background as sufficient criteria to indicate visibility impairment and will contest any who make such a claim. To demonstrate good faith and concern for appropriate scientific methods, Project MOHAVE

will arrange for tracer data to be withheld from all who have any role in attribution analysis until such time as physically meaningful empirical source attribution formulisms have been developed based upon other Project MOHAVE data. This will be done to promote the development of physically reasonable models prior to the availability of tracer data, and to avoid the appearance of forcing the models to fit preconceived notions.

Deterministic Meteorological Modeling

Deterministic meteorological modeling is based on fundamental physical conservation relationships. These relationships include conservation equations for momentum, temperature, mass, and the three phases of water. Meteorological modeling for Project MOHAVE will be done by Colorado State University using the Regional Atmospheric Modeling System (RAMS). A brief overview of RAMS is given in Appendix 6. Additional information about RAMS appears in Pielke *et al.*, (1990). A dedicated super workstation (IBM RISC) will be used for the modeling. The model will provide detailed wind and turbulence fields and a prediction of cloud height and location. Cloud predictions will be checked against satellite photographs.

The meteorological domain for the simulations will cover the southwestern United States. To obtain better terrain resolution near MPP, a telescoping nested grid will be used. In a nested grid approach, the larger scale results provide the boundary conditions for input into a finer scale modeling domain. The entire one year study period will be modeled. For selected cases from the intensive study periods, modeling with much finer resolution will be done. The preliminary grids to be used for the analysis are shown in Figure 10. Grids 1 and 2 will be used for the year-long study; the case studies will also use grids 3, 4, and 5. The horizontal and vertical number of grid points, and the horizontal grid spacing for each grid are shown below.

Grid	**# of grid points**			**Spacing (km)**
Grid 1	x=100	y= 60	z=44	32
Grid 2	x=104	y= 72	z=44	8
Grid 3	x=144	y=144	z=44	2
Grid 4	x= 80	y=80	z=44	0.5
Grid 5	x= 80	y=80	z=44	0.5

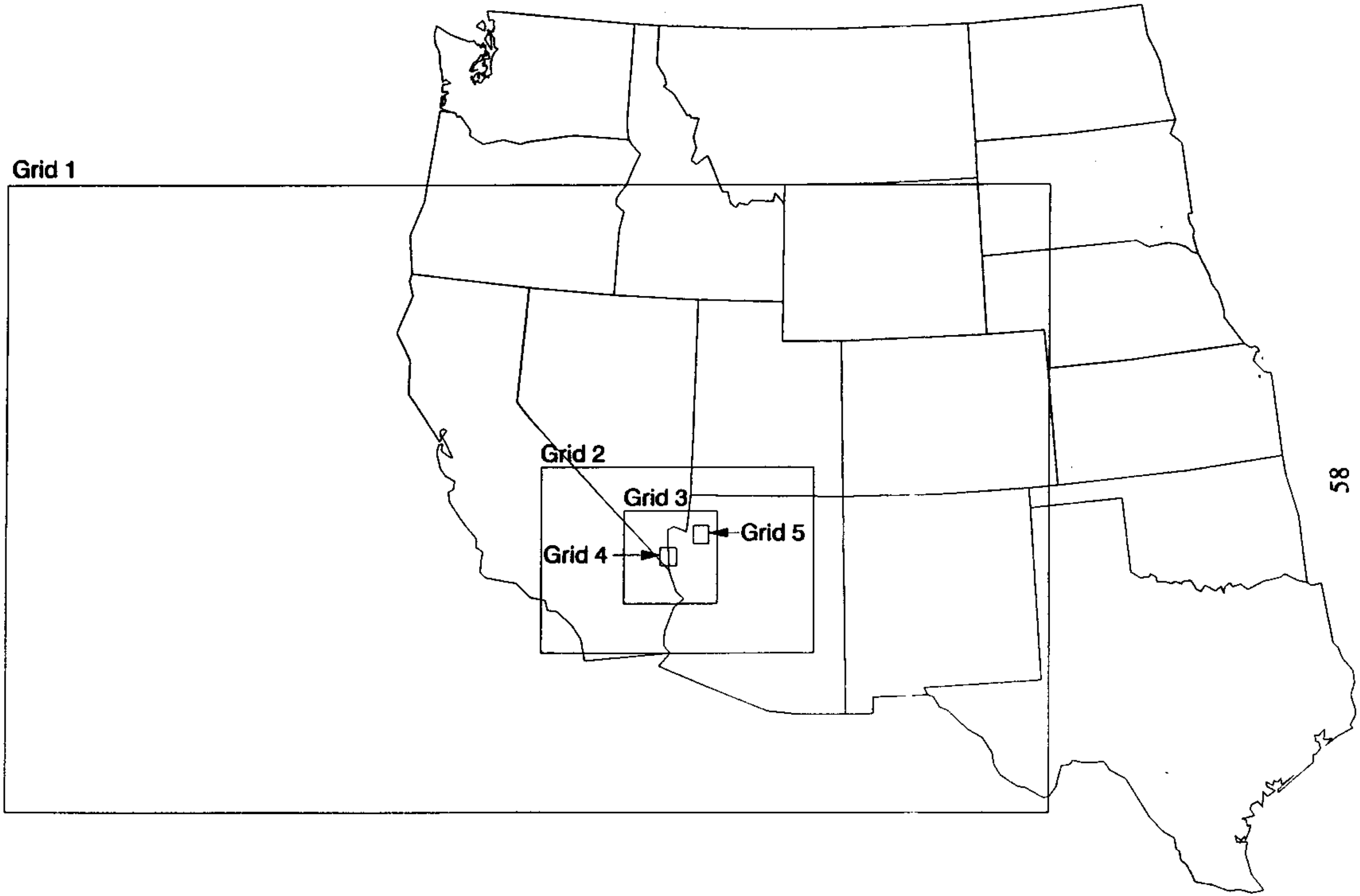

Figure 10. Meteorological modeling grid.

The model is initialized every 12 hours using the analysis field supplied the National Meteorological Center's Nested Grid Model. The Nested Grid Model uses surface and upper air data to generate initial fields of variables such as pressure, temperature, moisture and wind. The CSU RAMS modeling takes this initial field and generates mesoscale fields for the next 12 hours before being re-initialized.

The use of data from the wind profilers will be investigated for use in four-dimensional data assimilation. In this mode, the measured data are used to adjust, or "nudge" the model results. Data from the profiler site at Truxton are the most likely to be used for nudging. The Truxton site is in relatively open terrain and more likely to be representative of general flow in the study area than the other sites which are expected to be considerably influenced by local terrain features. Data from the radar wind profilers not used in the nudging process will be used to evaluate the performance of the model. The evaluation will be done for every hour having modeled and wind profiler data. A quantitative comparison between the predicted and observed winds will results in "figures of merit" for model predictions as a function of meteorological conditions. The wind and turbulence fields obtained from the deterministic meteorological model will provide the necessary input to calculate the transport and dispersion of MPP and other emissions of interest.

Transport, Chemical and Deposition Modeling

Once the wind fields have been determined, a model is needed to account for transport, chemical transformation and deposition. The transport model to be used is a version of the CAPITA Monte Carlo model currently being developed for EPA under a cooperative agreement with Washington University in St. Louis. A copy of the cooperative agreement proposal, which describes the modeling approach in more detail, appears as Appendix 7. The model is being developed specifically for visibility related studies. Evaluation and calibration of the model is being done using data sets such as IMPROVE, SCENES and NESCAUM. Modifications to the model to fully utilize the wind, turbulence, and moisture field supplied by the meteorological model may be necessary.

In the modeling approach, simulated pollutant quanta (particles) are "emitted" from each source. These quanta are moved in fixed time increments using wind fields supplied by the meteorological model. During transport the pollutant quanta are subject to chemical transformation and removal. The dispersion is achieved by imposing a randomized perturbation to the trajectory at each time step. Transformation and removal are also imposed as stochastic events at each time step. The result of the Monte Carlo simulation is a large number (10^5-10^6) of pollutant "particles" dispersed geographically for every time step of the simulation. The model is considered a Monte Carlo simulation because of the probabilistic treatment of transport, transformation, and removal.

The model will make use of the turbulence field generated by the meteorological model to perturb the trajectory. The moisture fields given from the meteorological model will be used to select between wet (heterogeneous) and dry (homogeneous) conversion rates in the SO_2 to sulfate transformation parameterization. Details of the modeling methodology are still to be determined. The model is based on that described by Patterson *et al.* (1981).

Hybrid and Receptor Modeling

Measurements of endemic and artificial tracers will be used to estimate the transport and dispersion of MPP and other sources. The transport can be verified by checking with trajectories given by the meteorological model. The transformation and deposition of SO_2 and sulfate are also necessary; these may be parameterized based upon such information as solar radiation, moisture (especially clouds), oxidant availability, and vertical mixing. The hybrid models will use tracer measurements to account for transport and dispersion, and parameterizations to account for deposition and transformation.

Versions of the chemical mass balance (CMB), differential mass balance (DMB), and possibly the tracer mass balance regression (TMBR) models will be used. CMB uses the relative ratios of natural or man-made tracers at the sources and receptor locations to apportion primary species for each measurement period. CMB will be used to apportion primary species using the high volume dichotomous sampler data. DMB, a hybrid model, uses trace material to establish dispersion factors and calculates the effects of deposition and oxidation. TMBR uses the variation of trace material over time to estimate primary or secondary aerosol contributions from each source. In its original formulation, TMBR requires a constant tracer to SO_2 emission ratio. However, Project MOHAVE will use a tracer emission rate that will be only approximately proportional to SO_2 emissions. TMBR may be used in an exploratory mode to investigate the effect of departure from model assumptions. Any use of the results must acknowledge and quantify the effects of departure from the model assumptions.

In DMB and TMBR it is assumed that each source has a uniquely emitted tracer associated with it. The best available emissions and source characterization data will be used to identify unique tracers for each significant source. If unique tracers are not available, CMB may be applied first to partition the ambient species concentrations into components attributable to the various groups of sources.

The NAS review of WHITEX noted a number of concerns about the use of DMB and TMBR. A summary of the NAS WHITEX comments and the steps that will be taken by Project MOHAVE to help resolve these issues appears as Appendix 8. The DMB and TMBR models will be modified to help alleviate concerns in the NAS review of WHITEX by taking advantage of the more detailed meteorological fields generated by the meteorological modeling that is a part of Project MOHAVE. For example, the effect of moisture upon conversion rates for both DMB and TMBR will utilize the moisture fields generated by the meteorological model.

As mentioned above, the implementation of DMB will differ from WHITEX by incorporating physical processes in a more robust manner. In Project MOHAVE, the effect of moisture on sulfate formation will be treated more rigorously than in the WHITEX study. In addition to surface moisture measurements, the deterministic meteorological model will give calculations of moisture at many vertical levels. This information will include prediction of clouds, which can be compared to satellite photos and surface observations. Rather than scaling linearly with surface relative humidity, the probability of plume-cloud interaction will be estimated and used to assign an SO_2-to-sulfate conversion rate. Rates of sulfate formation occur rapidly in clouds, and much slower without clouds. Different conversion rates based upon whether or not clouds are present should more appropriately account for the effect of moisture on conversion rates.

In DMB, as currently formulated, deposition and conversion rates are constant; the assumed rates are multiplied by plume age to give sulfate concentrations and deposition loss. Trajectory calculations are used to give plume age. Dispersion is accounted for by ratioing ambient trace material concentrations attributable to a source by known trace material release rates.
In Project MOHAVE variable conversion rates will be used, such as described above. With the deterministic meteorological modeling wind fields, reliable plume age calculations should be possible.

The equations for, and assumptions used in, CMB, DMB, and TMBR as presently formulated are given in Appendix 9.

Extrapolation of Intensive Study Periods to the Long-Term

To determine longer term impacts to visibility at GCNP, it is necessary to extrapolate from results of the intensive study periods. This will be a two-step process; the first step will relate the entire 12 month study period to the intensive period, while the second will extrapolate from the 12 month period to a multi-year period. The first step involves application of source-oriented and hybrid models, which will be developed and evaluated with intensive period data, to the meteorology and air quality data for the entire study period. In the second step the relative frequency of long-term meteorological patterns will be compared with those of the study period.

Deterministic models will be evaluated and calibrated using the more complete data of the intensive periods. The resulting models will then be run with data from the entire study period. For all modeling analyses a portion of the data may be withheld in order to independently test the models.

During the intensive study periods, hybrid modeling will use the artificial tracer results for MPP and any other sources tagged with artificial tracers. Hybrid models will also use endemic tracers for the remaining significant sources.

Results from hybrid models based on endemic tracers will be compared to results of the same models using artificial tracers to evaluate the utility of endemic tracers. If successful, models using endemic tracers will then be applied to the entire study period (covering a complete annual cycle) and used in conjunction with the deterministic modeling analysis.

The representativeness of the study year to longer term average conditions will be studied. It should be acknowledged that significant year to year variability in meteorological conditions occurs and that the likelihood of any given year being "typical" is not high. The frequency of occurrence of each meteorological regime identified in the meteorological classification process described in Section 11 will be compared for the study year and other years for which data are available. Where they exist, optical and air quality measurements from previous years will be compared to the study year measurements. The frequency of occurrence of each pattern for the study period and longer term average can then be compared to put the study year into perspective.

MPP Emission Modulation Study

The MPP was inoperative for a seven month period from July to December 1985. This presents a unique opportunity for investigating the effects of MPP. The MPP emission modulation study, discussed in Section 2 and Appendix 5 is a potentially powerful receptor approach to estimate the extent of MPP contributions to downwind sulfate levels. The analysis will be conducted by using a meteorological classification scheme to control for year-to-year variations in meteorology, and comparing measured sulfate at Spirit Mountain, Meadview and Hopi Point for periods of varying MPP and other SO_2 emissions. The study will include the following elements:

Independent statistical analysis of the experiment.

Chemical analysis of all filters. (Quality assurance will be evaluated through comparison of current results to past data through regression and time series analysis).

Classification of the synoptic and mesoscale weather patterns (meteorological regimes) affecting transport of the MPP plume.

Deterministic wind field, transport, and dispersion modeling for each of the meteorological regimes.

A detailed compilation of regional SO_2 emissions data for the control and outage period to allow an accounting for variation in SO_2 emission patterns.

All data manipulation will be performed in the "blind" to avoid charges of bias or data selection. Results of the study will be used along with the modeling and other analyses to estimate the effect of MPP on visibility at GCNP.

Framework for Interpreting Results

In a complex program such as this, a sound plan for compilation of results is as important as the collection of high quality and representative data and the performance of appropriate interpretive analysis. Development of an approach to organize the results from this program helps to focus attention and resources on critical steps for the entire program and communicate those ideas to others.

Just as it is inappropriate for worst case results to receive primary attention, it is also inappropriate to dwell on average or typical conditions, especially for an instantaneous effect such as visibility. The 12 month study period with hourly deterministic model results requires some method for summarizing the results of the study that avoids these pitfalls. A preliminary conceptual framework for summarizing the results of Project MOHAVE is shown in the table on the following page. The key idea is the stratification of time periods based upon

the locations with respect to GCNP of MPP emissions and those of other significant sources, such as from southern California. These would be based upon the modeling studies. Another stratification is whether the plumes have undergone wet or dry chemistry (based upon modeling results and observations). If useful, other stratifications could be developed. The frequency of each condition, the average and standard deviation of the percent sulfate from MPP, the percent of extinction from MPP and a measure of the perceptibility of the MPP impact is estimated for the study period.

Extrapolation to a long-term average will be done through the use of a meteorological classification scheme as previously described. This type of approach provides an efficient manner of presenting the magnitude and frequency of estimated MPP emissions on GCNP over a long-term period that could be used to evaluate the significance of existing impairment.

Conceptual Framework for Summarizing Project MOHAVE Results

GCNP Impact & Condition	Frequency (Deterministic Model)	% Sulfate (Reconciled Models)	% Extinction (Extinction Budget)	Measure of Perception
No MPP in GCNP				
MPP & SCA Dry				
MPP & SCA Wet				
MPP & Other Sources Dry				
MPP & Other Sources Wet				
MPP Alone Dry				
MPP Alone Wet				
Other Appropriate Categories				

SCA refers to the urban and industrial areas of southern California.

12. Overall Quality Assurance

Approach

An independent quality assurance audit will be done by ENSR. The major emphasis of independent quality assurance in Project MOHAVE will be upon verifying the adequacy of the participants' measurement procedures and quality control procedures, and upon identifying problems and making them known to project management. Although routine audits will play a role, major emphasis will be placed upon the efforts of senior scientists in examining methods and procedures in depth. This approach will be followed because fatal flaws in experiments emerge not from incorrect application of procedures by operators at individual sites or laboratories, but rather from incomplete procedures, inadequately tested methods, deficient quality control tests, or insufficient follow-up of problems.

System Audits - Study Planning and Preparation

Senior auditors will review study design documents to ensure that all measurements are being planned to produce data with known precision and accuracy. The auditors will verify that adequate communications exist between measurement and data analysis groups to ensure that measurements will meet data analysis requirements for precision, accuracy, detection limits, and temporal resolution. Quality control components of the measurements will include:

Determination of baseline or background concentrations and their variability.

Tests for sampler contamination.

Adequate and precise measurement of aerosol and tracer sampler volume and time.

Blank, replicate, and collocated samples.

Assessment of lower quantifiable limits (LQL), and determination of measurement uncertainty at or near the LQL.

Regular calibrations and calibration checks, traceable to standard reference materials.

Procedures for collecting QC test data and for calculating and reporting precision and accuracy.