DOE/EV-0008/2

The Multistate Atmospheric Power Production Pollution Study

Program Plan

(Addendum: Project Listings for FY-1977)

Sponsored by;

U.S. Department of Energy

Assistant Secretary for Environment

Division of Biomedical and Environmental Research

January 1978

DISCLAIMER

DOE/EV-0008/2
UC-11 & UC-90

MAP3S: STUDYING THE TRANSPORT, TRANSFORMATION AND FATE OF ATMOSPHERIC ENERGY-RELATED POLLUTANTS

ADDENDUM: PROJECT LISTINGS FOR FY 1977

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October 1977

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FOREWORD

The Multistate Atmospheric Power Production Pollution Study (MAP3S) is sponsored by the Assistant Secretary for Environment of the United States Department of Energy. The goal of the MAP3S program is to develop and demonstrate an improved, verified numerical capability to simulate the present and potential future changes in pollutant concentration, atmospheric behavior and precipitation chemistry as a result of pollutant releases to the atmosphere from large scale power production processes, primarily coal combustion. The research required to meet this goal has been described in the MAP3S Plan. This first annual addendum to the plan contains a listing of individual projects that are sponsored by MAP3S, both those on which progress can be reported based on work in FY-1976 and early FY-1977 and those being planned for FY-1977 and beyond.

Taken together, we expect these research projects and those related activities sponsored by the U. S. Environmental Protection Agency, the Electric Power Research Institute and other organizations, to provide the needed basis for an improved assessment of the impact of emissions of atmospheric energy-related (AER) pollutants from fossil fuel energy generation. Annual updates for these listings will be issued in order to provide an outline of the continuing program. The detailed research results will be presented in the technical literature and in further MAP3S reports, as appropriate.

The appendix lists the abbreviations of organizations referred to in this report.

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SECTION 1

MAP3S BRIEF PROJECT REPORTS

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TASK 1: Power Production Emissions

SUB-TASK: 1. Source Characterization

CONTACT: R. N. Dietz, S. E. Schwartz, BNL

OBJECTIVE: Determine and characterize sulfate, sulfuric acid, and particulate emissions from fossil-fueled sources.

RESEARCH ACTIVITIES: An extensive review of the literature relevant to the characterization of source emissions and the effect of the important controlling parameters has been performed. In addition, a detailed review of the sampling and analytical procedures resulted in the selection of in-stack filtration and controlled condensation for initial field evaluation.

The method has been demonstrated in our laboratory to be greater than 95 percent effective for determining sulfuric acid with negligible error (less than 0.3 ppm) from conversion of SO_2 to acid. A total of 20 field sampling runs at a nominal 400 MW_e oil-fired power plant showed that from the electrostatic precipitator controlled unit, sulfuric acid concentration was typically 2 to 5 ppm; sulfate, 3 to 8 ppm; and SO_2, 1430 to 1500 ppm. Thus, the total sulfate species emitted ranged from only 0.3 to 1% of the sulfur in the fuel. Reliability of the technique is based on excellent material balance for total sulfur and total water. Emissions increased linearly with excess furnace oxygen and exponentially with power level.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: BNL, EPA, EPRI, LILCO

REFERENCES:

Dietz, R. N. and R. F. Wieser, "Sulfate Emissions from Fossil Fueled Combustion Sources," Semi-annual Report No. 4, February 1977.

TASK 1: Power Production Emissions

SUB-TASK: 2. Emissions Inventory Compilation

CONTACT: C. M. Benkovitz, BNL

OBJECTIVE: Compile "best-estimate" emissions inventory.

RESEARCH ACTIVITIES: Initial emissions data were obtained by BNL's Regional Energy Studies Program from EPA's National Emissions Data System inventory early in calendar 1976. A prototype computerized data base of point source information has been designed and loaded covering the northeastern United States (Virginia/West Virginia, Pennsylvania to Maine and the Atlantic Ocean). Data is disaggregated to the point source level and includes TSP, SO_2, NO_x, HC and CO emissions, stack information (diameter, height, flow rate), plant scheduling information and plant operating characteristics.

Preliminary studies of the data have concentrated in developing computer methodologies and criteria with which to undertake quality assessment studies. Methodologies to format this data for input to models are also being developed.

Federal Power Commission (FPC) form 67 data have been obtained and are being evaluated for inclusion in the computerized inventories. State and local agencies are being contacted to obtain additional data and, when obtained, such data are being studied and merged with NEDS data.

Studies of area source emissions data have clearly demonstrated the need for additional geopolitical data - notably cross reference lists of state/county codes in use by different agencies and census-type information (population and geographic data). Such data are being assembled.

Methodologies for handling geocoded data are being studied and whenever applicable, are being developed to facilitate handling of emissions inventory data. Examples of such methodologies are gridded procedures, grid-to-grid transformations and polygon/grid studies.

REPORTING ORGANIZATION: Brookhaven National Laboratory

TASK 2: Nonpower Production Emissions

SUB-TASK: 1. Smelter Plumes, Sudbury

CONTACT: L. Newman, J. Forrest, BNL

OBJECTIVE: Measurement on Plume Components for Conversion Studies.

RESEARCH ACTIVITIES: The plume data obtained on the extent of oxidation of sulfur dioxide to sulfate from the Sudbury smelter operation were interpreted as arising from a heterogeneous catalytic pseudo second-order mechanism. The rate of reaction was found to be 0.2 $ppm^{-1}\ h^{-1}$. This value is 1/5 that found for the pseudo-second-order constant at an oil-fired plume. Of significance to a heterogeneous mechanism was that the emitted particulate loading of 0.04 grams per liter of emitted sulfur dioxide at the smelter operation was low but possibly only coincidentally equal to 1/5 that of the oil-fired operation.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: Atmospheric Environment Service (Canada)

REFERENCES:

Forrest, J. and L. Newman, "Oxidation of Sulfur Dioxide in the Sudbury Smelter Plume," *Atmos. Environ.*, 1977 (in press).

TASK 3: Pollutant Properties

SUB-TASK: 1. Analytical Methods Development

CONTACT: Roger L. Tanner, BNL

OBJECTIVE: Development and application of trace analytical methods for determination of sulfur-related pollutants.

RESEARCH ACTIVITIES: The Gran titration method was optimized and routinely applied for determination of strong acid in airborne particles, the data base indicating a significant correlation of acid and sulfate in fine fraction particles but also showing the confounding presence of strong base materials in coarse fraction particles. Extraction techniques for sulfuric acid and bisulfate have been further developed and appear adequately sensitive and precise for hourly HiVol airborne particle samples. The flash volatilization-flame photometric technique for ng quantities of soluble sulfur has been optimized and, although recoveries are not always 100%, appears highly suited for determination of extracted H_2SO_4 and bisulfate samples. Preliminary investigation of instrumentation for real-time aerosol analysis indicates adequate sensitivity is available for aerosol sulfate concentrations down to 2 $\mu g/m^3$. Comparison of soluble sulfur, sulfate and total sulfur data for airborne particle samples, in addition to indicating that > 90% of total aerosol sulfur is present as sulfate, has also been useful in identifying preferred methodology for various proposed experiments. Experiments have demonstrated inertness of treated quartz filters (and aged aerosol samples collected thereupon) to artifact sulfate formation by SO_2 oxidation.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Tanner, R. L., et al., "Separation and Analysis of Aerosol Sulfate Species at Ambient Concentrations," *Atmos. Environ.*, *11*, 955, 1977.

TASK 3: Pollutant Properties

SUB-TASK: 2. Aerosol Measurement

CONTACT: W. H. Marlow, BNL

OBJECTIVE: Development of aerosol instrumentation, associated analytical methods, and the theory of aerosol measurement.

RESEARCH ACTIVITIES: To fill the void of instrumentation capable of providing size-related separations for chemical analysis of suboptical aerosol particles, "diffusion processing" of aerosols has been introduced under this project. The method has essentially no practical limitations on the volume of aerosol that can be sampled and it does not suffer from ambiguities due to probable physical and chemical transformations of the sampled aerosol that possible low pressure and electrical charging methods have.

To assess deviations of diffusion processing from ideal behavior, fractional penetrations of optical-range particles, through elements of the processor have been measured.

A high volume, airborne, aerosol sampling system for dedicated use in the BNL MAP3S airplane has been designed and is currently under construction. It will draw a total volume of over 200 l.p.m. to allow individual filter samples from the source. The sampler consists of three stages: (1) dichotomous virtual impactor with 2 μm cut point; (2) slit-to-cylinder impactor with approximately 0.5 μm cut; (3) diffusion processor with nominal 0.05 μm cut.

In collaboration with DOE's Environmental Measurements Laboratory, a general method making no assumptions concerning form of the distribution for the extraction of aerosol size distribution information from calibration and measured data has been developed and employed.

Calculations of time-dependent, polydisperse aerosol charging by polydispersions have been performed. They have delineated the domains of validity of aerosol measurement methods which rely upon diffusion charging and replaced the conventional parameterization ("$N_o t$") for aerosol charging by a more generally valid one.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATION: EML

REFERENCES:

Marlow, W. H. and R. L. Tanner, "Diffusion Sampling Method for Ambient Aerosol Size Discrimination with Chemical Composition Determination," *Anal. Chem.*, *48*, 1999, 1976.

Marlow, W. H., "Calculations of Unipolar Aerosols Charging," *Interface Science, Vol. II: Aerosols, Emulsions and Surfactants*, Milton Kerker (Ed.), Academic Press, 211, 1976.

Marlow, W. H., "A Limitation on Electrical Measures of Aerosols," presented at Eighth Materials Research Symposium, Methods and Standards for Environmental Measurement, Gaithersburg, Maryland, September 20-24, 1976.

Marlow, W. H., "Optical-Size Particle Penetration Through a Diffusion Processor for Filter Sampling," presented at the Conference on Industrial Hygiene, New Orleans, LA, May 23-27, 1977.

Marlow, W. H., "Unipolar Aerosol Diffusion Charging, I: Introduction and Charging of High and Low Dielectric Constant Monodisperse Aerosols by Time-Invariant Ion Distributions," *J. Colloid Interface Sci.* (in press).

Marlow, W. H., "Unipolar Aerosol Diffusion Charging, II: Ion and Aerosols Polydispersities in Unipolar Charging the 'Diffusion Charging Mobility Analysis' Hypothesis," *J. Colloid Interface Sci.* (in press).

TASK 3: Pollutant Properties

SUB-TASK: 3. Size Distributions of Airborne Elements

CONTACT: Donald F. Gatz

OBJECTIVE: To determine the variation with particle size of atmospheric elements and ions in the St. Louis area.

RESEARCH ACTIVITIES: Twenty-eight sets of cascade impactor samples collected in 1972, 1973 and 1975 from seven different sites in the St. Louis area were analyzed for Li, Na, Mg, K, Ca, Fe, Mn, Zn, Cd, and Pb. Six additional samples from 1971 were analyzed for $SO_4^=$. The 1971 samples used thin polyethylene discs as impaction substrates, whereas Whatman-41 filter paper substrates were used for the rest of the samples. The results show that the elements analyzed fall into three general size classes: large, having most mass on particles with diameters larger than about 3 μm; small, having most mass on particles with diameters less than 1 μm; and a mixed category, having contributions from both large and small size classes. Elements falling in the large particle category include Li, Mg, Ca, and Fe; these are believed to be primarily soil-derived. Small-particle species include Zn, Cd, Pb, and $SO_4^=$; these are mainly anthropogenic. Elements K, Na and Mn are in the mixed category.

REPORTING ORGANIZATION: Illinois State Water Survey

COOPERATING ORGANIZATIONS: State of Illinois; NSF/RANN; EPA; ANL; PNL; University of Chicago; University of Wyoming; SRI, International; NOAA.

REFERENCES:

Gatz, D. F., "Airborne Elements: Their Concentration Distributions at St. Louis," in *Study of Air Pollution Scavenging: Fifteenth Progress Report*, Illinois State Water Survey Report COO-1199-58, 1977.

TASK 3: Pollutant Properties

SUB-TASK: 4. Aerosol Source Identification: Factor Analysis of Elemental Composition Measurements

CONTACT: Donald F. Gatz

OBJECTIVE: To identify major sources of airborne elements in the St. Louis area.

RESEARCH ACTIVITIES: A set of 400 aerosol samples was collected on Nuclepore filters at 12 sites in the St. Louis area during summers from 1973 to 1975. The filters were analyzed for 11 elements by ion-excited x-ray fluorescence at the University of California - Davis. The data at each site have been analyzed separately using factor analysis and derived factors interpreted as aerosol sources. Results from the various sites consistently identify the following major sources (percentages in parentheses give contributions of each source to observed total aerosol concentrations): (1) soil, dust and flyash (10-30%), (2) secondary sulfates (20%), (3) metals processing (10%), and (4) auto exhaust (2-6%). In addition, minor sources of Ti (a pigment plant) and Pb (a secondary lead smelter) were identified. Major sources of Ti and Pb in the St. Louis area are soil dust and auto exhaust, respectively.

REPORTING ORGANIZATION: Illinois State Water Survey

COOPERATING ORGANIZATIONS: State of Illinois; NSF/RANN; EPA; ANL; PNL; University of Chicago; University of Wyoming; SRI, International; NOAA.

REFERENCES:

Gatz, D. F., "Aerosol Source Identification and Reconciliation in METROMEX," in *Study of Air Pollution Scavenging: Fifteenth Progress Report*, Illinois State Water Survey Report COO-1199-58, 1977.

TASK 4: Pollutant Distribution

SUB-TASK: 1. MAP3S Experimental Sampling Network Design

CONTACT: C. M. Sheih and B. B. Hicks

OBJECTIVE: To provide criteria for the selection of regional-scale experimental sites, sampling times, and sampling intervals.

RESEARCH ACTIVITIES: Field experiments employing a network of sampling stations are classified into two categories, according to whether the aim is to investigate the mechanisms of atmospheric pollutant transformation and transport (a "tracer" experiment) or to evaluate the extent of air pollution (an air quality monitoring experiment). Optimal distributions of surface sampling stations, sampling times, and sampling durations have been deduced.

REPORTING ORGANIZATION: Argonne National Laboratory

REFERENCES:

Sheih, C. M., G. D. Hess, and B. B. Hicks, "Design of Network Experiments for Regional-Scale Atmospheric Pollutant Transport and Transformation," in Preprints Volume of the *AMS/APCA Joint Conference on Applications of Air Pollution Meteorology*, November 29-December 2, 1977, Salt Lake City, Utah (also *Atmospheric Environment*, 1978, in press).

TASK 4: Pollutant Distribution

SUB-TASK: 2. Objective Network Analysis

CONTACT: J. D. Shannon and M. L. Wesely

OBJECTIVE: Optimize a ten sensor pyranometer network in order to observe regional scale turbidity across the MAP3S area, with emphasis on the adequate detection and mapping of episodes of high turbidity.

RESEARCH ACTIVITIES:

1. Correlation coefficients between past observations of turbidity in and around the Northeast have been calculated for various levels of turbidity.
2. A correlation structure function (CSF) has been fitted to the correlation coefficients by nonlinear programming (NLP) techniques.
3. Proposed sensor networks have been evaluated through the use of the CSF in modeled objective analyses; the distribution of sensors has been optimized by the use of NLP techniques.
4. The relative value of adding extra stations has been calculated objectively.
5. The optimized pattern has been used as a guide for actual sensor location, which must meet site, power, and servicing requirements.

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATIONS: University of North Dakota, Department of Aviation.

REFERENCES:

Shannon, J. D., M. L. Wesely and P. J. Brady, "Objective Sensor Placement for Sampling Regional Turbidity," *Atmos. Environ.* (in press), 1978.

Shannon, J. D. and M. L. Wesely, "Objective Placement of Sensors for a Regional Turbidity Network," *Proceedings of the 5th Conference on Probability and Statistics in the Atmospheric Sciences*, November 1977.

TASK 4: Pollutant Distribution

SUB-TASK: 3. Vertical Pollution Distribution

CONTACT: R. W. Garber, R. M. Brown, and S. E. Schwartz, BNL

OBJECTIVE: Determine vertical distribution of pollutants as a function of meteorological conditions.

RESEARCH ACTIVITIES: Fifteen vertical transversing experiments have been made during early 1977 over central Long Island to determine the temporal variability of nephelometric total suspended particulates, SO_2 and $SO_4^=$. The measurements were made from 300 to 3000 meters in altitude under varying atmospheric conditions. Temperature profiles and turbulence measurements (MRI-UITS system) were used to determine the stability as a function of altitude. The SO_2 and $SO_4^=$ measurements were made using a filter pack assembly and concentrations determined in the laboratory.

Preliminary results from these tests indicate in general that there is a steady decrease in all vertical concentrations when near adiabatic temperature conditions prevail but that abrupt changes are evident when temperature inversions exist. Sufficient data do not as yet exist to establish significant trends in ratios of total particulate to particulate sulfate or sulfur dioxide to particulate sulfate, although these ratios are being studied as more data become available.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Brown, R. M. and R. W. Garber, "Airborne Measurements of Aerosol and Sulfate Concentration Discontinuities in Vertical and Horizontal Profiles," *Proceedings of Third Symposium on Atmospheric Turbulence, Diffusion and Air Quality*, American Meteorological Society, pp. 340-343, 1976.

TASK 4: Pollutant Distribution

SUB-TASK: 4. Aircraft Operations

CONTACT: R. W. Garber, BNL

OBJECTIVE: Modify standard commuter type aircraft for atmospheric science studies.

RESEARCH ACTIVITIES: Obtained Britten Norman Islander aircraft on exclusive use lease and have completed installation of principal scientific equipment and instrumentation including:

1. Atmospheric Sampling System
   a. Isokinetic Probe for Hi Volume Sampler
   b. Isokinetic Probe for Particulate Size Discrimination Sampler
   c. Probe for Real Time Gas Monitors
2. Meteorological Monitoring Systems
   a. Temperature System
   b. Atmospheric Pressure Sensor
   c. Dew Point Monitor
   d. Turbulence Monitor
   e. UV and Total Solar Radiation Sensors
   f. Airspeed Indicator
3. Navigational Data System
   a. Doppler Radar System - Ground Speed and Drift Angle
   b. Distance Measuring Equipment
   c. VOR Direction Indicators
   d. Gyrocompass
4. Gas Monitoring Equipment
   a. Flame Photometric Sulfur Monitor
   b. Chemiluminescence NO-NO_x Monitor
   c. Chemiluminescence O_3 Monitor
5. Particulate Monitoring Equipment
   a. Condensation Nuclei Counter
   b. Integrating Nephelometer
   c. Particulate Size Discrimination
   d. Sampler System

6. Sample Collection Systems
    a. Hi Volume System
    b. Size Discriminated Particulate Sample System
7. Other Equipment
    a. Real Time Data Collection System
    b. Electrical Power Converters
    c. Pumps for Air Samplers

All equipment has been tested in the laboratory by both static operations and simulation of field studies. Systems are undergoing extensive in-aircraft testing and calibration. Initial airborne calibration runs are scheduled for June and early July 1977.

TASK 5: Pollutant Transport

SUB-TASK: 1. 1976 "Sangamon" PBL Profile Studies

CONTACT: B. B. Hicks

OBJECTIVE: To investigate the evolution of the nocturnal inversion in well-documented and easily-understood circumstances, with the intent of developing parameterization procedures suitable for inclusion in numerical simulations.

RESEARCH ACTIVITIES: During a two week period of July 1976, an intensive investigation of the growth of the nocturnal inversion took place over mixed soybean and corn fields in Sangamon County, near Springfield, IL. Hourly radiosonde ascents, tracked by the double-theodolite WHAT system to give better than ten meter resolution on both wind and temperature, and interspersed kytoon soundings using faster response instrumentation were used to detect and study the stable layers that occur in the night-time atmosphere near the surface. Supporting surface observations of standard meteorological properties were made continuously, together with eddy flux measurements during much of the period. A network of microbarographs on a 200 km base was used to obtain geostrophic data; in order to assure accuracy, each station was visited at regular intervals.

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATIONS: EPA, PNL, ISWS, University of Minnesota, University of Michigan, Florida State University, Pennsylvania State University.

REFERENCES:

Sisterson, D. L., B. B. Hicks, and M. L. Wesely, "An Outline of the 1976 Sangamon Field Experiment," *Annual Report, Argonne National Laboratory, Radiological and Environmental Research Division*, ANL-76-88, Part IV, p. 1-6, 1977.

Sisterson, D. L. and P. Frenzen, "Nocturnal Boundary-Layer Wind Maxima and the Problem of Wind Power Assessment," *Environ. Sci. and Tech.*, 1978 (in press).

TASK 5: Pollutant Transport

SUB-TASK: 2. Planetary Boundary Layer Acoustic Sounding Studies

CONTACT: E. L. Miller and B. B. Hicks, ANL

OBJECTIVE: To monitor the evolution of the tropospheric mixed layer in order to improve the parameterizations of vertical dispersion used in numerical models, and to study the spatial variability of the PBL.

RESEARCH ACTIVITIES:

1. During July 1976, an array of acoustic sounders was set up in conjunction with the ANL "Sangamon" study of PBL behavior. A baseline of about 1.5 km was used in order to look at such phenomena as the phase velocity and wavelength of waves associated with nocturnal inversions.
2. An extensive period of observations made by use of a monostatic acoustic sounder located at ANL has been obtained. Periods of very shallow mixing depth have been selected for scrutiny by atmospheric chemists, looking for differences between air beneath a capping inversion and the overlying, decoupled air aloft.
3. Mobile acoustic sounders have been operated in conjunction with manned balloon flights conducted as part of the U. S. Department of Energy "da Vinci" program.

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATIONS: Sandia Laboratories, Florida State University, and others.

REFERENCES:

Miller, E. L., "Accoustic-Sounder Investigation of the Effects of Boundary Layer Decoupling on Long-Distant Pollutant Transport," *Annual Report, Argonne National Laboratory, Radiological and Environmental Research Division*, ANL-76-88, Part IV, p. 24-28, 1977.

TASK 5: Pollutant Transport

SUB-TASK: 3. Development of Long-Range Tracer System for Atmospheric Tracer Studies

CONTACT: G. J. Ferber, ARL

OBJECTIVE: To develop instrumentation and techniques for release, sampling, and analysis of perfluorocarbons and to determine the feasibility of their use in atmospheric dispersion experiments over distances from about 100 to 1000 km.

RESEARCH ACTIVITIES: Three prototype sampling devices have been developed for the perfluorocarbon system. Two of the devices are automated sequential samplers, one of which also performs an *in situ* analysis of perfluorocarbon concentration. The third device, designed for airborne sampling, provides continuous, in-flight read-out of air concentration. A full scale field test of the perfluorocarbon tracer system was conducted in Idaho in April. Two perfluorocarbon tracers (C_6F_{12} and C_8F_{16}) were released over a 3-hour period along with two heavy methanes and SF_6. In addition to the prototype samplers, more than 100 samples were collected at 3, 50 and 90 km. Samples will be analyzed for all five tracers to test the reliability of release, sampling and analysis procedures. The prototype sequential samplers appeared to perform well but the airborne instrument had serious problems requiring design modifications.

REPORTING ORGANIZATION: NOAA-Air Resources Laboratory

COOPERATING ORGANIZATIONS: EML, DNL

TASK 5: Pollutant Transport

SUB-TASK: 4. Measurement of Long-Range Tracer Compounds

CONTACT: R. N. Dietz, BNL

OBJECTIVE: Develop electron capture chromatographic techniques for unique tracer compounds and evaluate performance in multi-tracer release experiments.

RESEARCH ACTIVITIES: A very precise analytical chromatograph procedure for the determination of the atmospheric tracer compound, sulfur hexafluoride, has been developed and employed in several cooperative field experiments. With a limit of detection of about 0.01 parts per trillion parts of air, quantitative measurements (10 times ambient levels) at 100 km from the release point (50 to 80 pounds/hour of SF_6) have been made.

Long-range tracing (500+ km), which cannot be performed with SF_6 because of the current ambient levels ($\sim$ 0.5 ppt), can be accomplished with tracers having negligible ambient levels (0.01 to 0.001 ppt). Several substitute tracers from the perfluorocarbon family (perfluoro-dimethylcyclobutane, -monomethylcyclohexane, and -dimethylcyclohexane) have been selected for preliminary field evaluation.

Accurate standards at 10 ppt have been prepared for each tracer and an analytical scheme for the simultaneous chromatographic determination of the 3 perfluorocarbons and SF_6 has been developed. The data from a field experiment performed in conjunction with NOAA and EML will provide an evaluation of the capability of each of the tracers. A portable continuous monitor with 1 ppt detectability was developed.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: EML, ARL

REFERENCES:

Dietz, R. N., E. A. Cote and R. W. Goodrich, "Ultratrace Determination of Sulfur Hexafluoride and Perfluorocarbons for Atmospheric Tracing," ACS Meeting, Chicago, IL, August 1977.

Dietz, R. N., E. A. Cote and R. W. Goodrich, "Air Mass Movements Determined by Real-Time Frontal Chromatography of Sulfur Hexafluoride," in *Measurement, Detection, and Control of Environmental Pollutants*, IAEA-SM-206/21, September 1976, pp. 277-299.

TASK 5: Pollutant Transport

SUB-TASK: 5. Trace-Metal Concentration Ratios as Indicators of Pollution Source

CONTACT: J. A. Young, PNL

OBJECTIVE: To determine whether interrelationships between trace metal concentrations from various urban areas can be used to "fingerprint" air masses having been polluted in those areas.

RESEARCH ACTIVITIES: Air filter samples have been collected by aircraft for trace element analysis downwind of 12 major U. S. cities to determine whether the trace element concentration ratios are sufficiently different between cities, and sufficiently constant for a given city, to make it possible to determine the source of the atmospheric contaminants at rural locations from the measured concentration ratios and the ratios characteristic of various urban-industrial complexes. Samples were collected downwind of St. Louis, Indianapolis, Columbus, Pittsburgh, Buffalo, Rochester, Allentown-Bethlehem, Philadelphia, Baltimore, Washington, D. C., and New York City in December 1974 and upwind and downwind of Kansas City, Indianapolis, Columbus, and Pittsburgh in June of 1975.

It was found that the trace element concentration ratios of anthropogenic elements generally varied the most. Between any two cities, there were generally several concentration ratios which were different by more than an order of magnitude. The differences in the ratios between different cities appeared to be much greater than the variation with time for a given city.

These results indicate that the plumes of different cities can be distinguished one from another using trace element ratios. However, more work needs to be done to determine the variability of the ratios characteristic of given cities with time, and to determine the net trace element ratios emitted by major cities.

REPORTING ORGANIZATION: Pacific Northwest Laboratory

REFERENCES:

PNL Annual Report for 1975 to USERDA Division of Biomedical and Environmental Research, Part 3, Atmospheric Sciences, BNWL-2000, Pt. 3, 1975.

TASK 6: Pollutant Transformation

SUB-TASK: 1. Airborne Plume Study

CONTACT: R. W. Garber, L. Newman, BNL

OBJECTIVE: Airborne measurement of plumes from fossil-fueled power stations.

RESEARCH ACTIVITIES: Conduct a series of studies with instrumented aircraft of fossil-fueled power station plumes. The principal objective is to build a data base to determine the chemical and physical behavior of these plumes and to ascertain conditions which affect their behavior. These studies will be principally conducted in the northeast region and will be preferentially directed toward oil-fired installations although some coal-fired installations will also be studied. The preference for the study of oil-fired systems is dictated by the prevalence of oil-fired power stations in the northeast region.

Currently plume studies are being conducted at the Northport Power Station at Northport, L.I. under an agreement with LILCO, EPRI and ESEERCO. To date approximately 10 experiments have been conducted and more are planned for the future.

Several experiments have been conducted at other power stations at locations including St. Louis, MO; Albany, N.Y. and Clearwater, FL. Extensive data sets have not yet been obtained; however, the results can be used for future experimental guidance. The data from the experiments conducted in the vicinity of Clearwater, FL show an apparent constant and low transformation of sulfur dioxide under most atmospheric conditions. Approximately 2% of the plume sulfur appears as sulfate independent of distance and both during daylight and dark conditions and under relatively high humidity. These results are counter to independent source measurements which indicate sulfate levels approaching 10% in the plant ducts prior to emission into the atmosphere. Several processes have been invoked to be tested.

Among the experiments to be performed will be observation of the effect of higher relative humidity on plume chemistry, the effect of plant

operational parameters on plume behavior and accounting for differences in source and plume measurements.

The first plume studies for MAP3S are scheduled for the Fall of 1977.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Forrest, J. and L. Newman, "Further Studies on the Oxidation of Sulfur Dioxide in Coal-Fired Power Plant Plumes," *Atmos. Environ., 11*, 465-474, 1977.

TASK 6: Pollutant Transformation

SUB-TASK: 2. Theoretical Analysis of Chemical Reactions in Stack Plumes

CONTACT: S. E. Schwartz, BNL

OBJECTIVE: Describe processes controlling fate and extent of in-plume oxidation of SO_2 in plumes from power plants and smelters.

RESEARCH ACTIVITIES: A formalism has been developed that treats chemical reactions in expanding stack plumes of arbitrary concentration profile to examine the effects of dilution and catalyst depletion upon SO_2 oxidation. The rate of plume expansion is shown to exert a controlling influence upon the rate and ultimate extent of reactions that are higher than first order in plume constituents. Quenching of chemical reactions is exhibited at high expansion rates and the conditions leading to quenching are established.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Schwartz, S. E. and L. Newman, "Processes Limiting the Oxidation of Sulfur Dioxide in Stack Plumes," *Environ. Sci. & Tech.* (in press), 1977.

TASK 6: Pollutant Transformation

SUB-TASK: 3. Long-Range Plume Transformation Study

CONTACT: A. J. Alkezweeny and J. M. Hales, PNL

OBJECTIVE: Determination of parameters describing pollutant transformations in urban plumes (and imbedded power plant plumes) for subsequent use in regional modeling efforts.

RESEARCH ACTIVITIES: The Long-Range Plume Transformation study is based near Lake Michigan, where the long run of plumes over the lake is used advantageously to provide large distances ($\sim$ 80 miles) for plume sampling over a highly uniform surface. Under these conditions, airflow is relatively simple and the competing effects of dry deposition are less difficult to account for in the data interpretation process.

The first field series of this study was performed in a three-week period during the summer of 1976. This experiment was conducted with the cooperative efforts of several groups besides Battelle-Northwest, including the University of Michigan (oxidant studies), NASA (CO remote sensing) and the EPA (hydrocarbon analysis). Two Battelle-Northwest aircraft were used in the experiment. The first of these was a DC-3, which is essentially fully instrumented with aerosol and trace gas monitoring equipment. This aircraft performed plume cross sections, and was complimented by a twin Cessna, which obtained off-plume SO_2 and sulfate measurements. A schematic depicting the study during one of the experiment days is shown in Fig. 1. Data from the summer 1976 experiments are currently being interpreted with the aid of a diagnostic reactive plume model. Experiences with this analysis will dictate modifications to be imposed on the field experiment during the coming year.

REPORTING ORGANIZATION: Battelle, Pacific Northwest Laboratories

COOPERATING ORGANIZATIONS: University of Michigan, EPA, and NASA

REFERENCES:

Hales, J. M. et al., "Pacific Northwest Laboratory Annual Report for 1976 to the ERDA Assistant Administrator for Environment and Safety," BNWL-2100 Pt. 3, 232 p., August 1977.

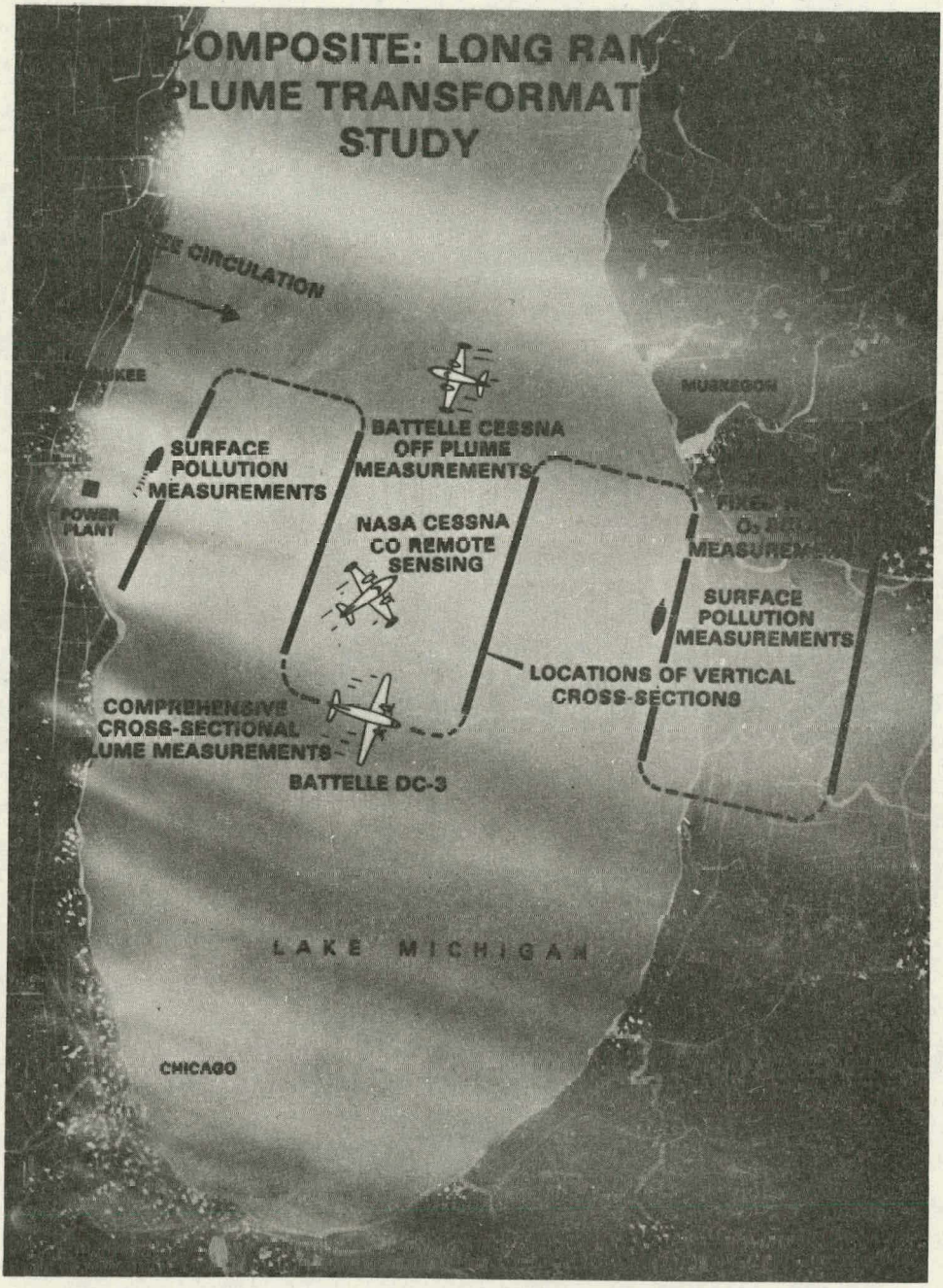
COMPOSITE: LONG RAN
PLUME TRANSFORMAT
STUDY
E CIRCULATION
MUSKEGON
BATTELLE CESSNA
OFF PLUME
MEASUREMENTS
SURFACE
POLLUTION
MEASUREMENTS
POWER
PLANT
NASA CESSNA
CO REMOTE
SENSING
SURFACE
POLLUTION
MEASUREMENTS
LOCATIONS OF VERTICAL
CROSS-SECTIONS
COMPREHENSIVE
CROSS-SECTIONAL
UME MEASUREMENTS
BATTELLE DC-3
LAKE MICHIGAN
CHICAGO

FIGURE 1.

TASK 6: Pollutant Transformation

SUB-TASK: 4. Milwaukee Urban Plume

CONTACT: Roger L. Tanner, BNL

OBJECTIVE: Study transport and transformation of pollutants in the Milwaukee urban plume.

RESEARCH ACTIVITIES: Airborne particles and SO_2 were collected on BNL-prepared quartz and carbonate-impregnated cellulose filters, respectively during airborne urban plume experiments in the Milwaukee area, August 1976. Particle samples have been analyzed for strong acid, ammonium, soluble sulfate nitrate and total sulfur. Sulfate levels are strongly correlated with ammonium in particle samples but unrelated to nitrate levels. The ratio of particulate sulfur (S_p) to total sulfur ($SO_2 + S_p$) does not vary downwind from Milwaukee in an interpretable fashion.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATION: PNL

REFERENCES:

Tanner, R. L., R. Cederwall, R. Garber, D. Leahy, W. Marlow, R. Meyers, M. Phillips and L. Newman, "Separation and Analysis of Aerosol Sulfur Species at Ambient Concentrations," *Atmos. Environ.*, *11*, 955, 1977.

TASK 6: Pollutant Transformation

SUB-TASK: 5. Urban Plume Studies by Diffusion Sampling

CONTACT: R. L. Tanner and W. H. Marlow, BNL

OBJECTIVE: To determine the chemical composition of airborne sulfate as a function of particle size in the range < 0.4 μm by diffusion sampling in urban, rural and intermediate regions; to intercorrelate chemical compositional parameters, particle size, air mass back-trajectories and emission sources and identify diurnal and seasonal variations in these correlation patterns.

RESEARCH ACTIVITIES: Experiments were conducted for 8 days in July 1975 at rural Glascow, IL, for 24 days in August 1976 and again in February 1977 in New York City and were supplemented by shorter duration experiments at BNL during 1975 and 1976. Proportions of aerosol sulfate, ammonium/sulfate and acid/sulfate ratios were determined as a function of particle size in the < 0.4 μm range. Although data anlayses are incomplete for the later experiments, some important implications have been documented: one episode of diurnal acid and ammonium concentration variation during the Glascow experiment was suggestive of photochemically induced H_2SO_4 formation, but generally no diurnal patterns could be discerned from the 12 hr sampling format; sulfate constitutes, as expected, a larger portion of suboptical (< 0.3 μm) aerosol volume than of larger particles; ammonium levels closely correlated to sulfate levels in both urban and rural samples independent of back-trajectory with an average NH_4^+/SO_4^{2-} molar ratio of 1.5 in New York City during August 1976.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATION: EML

REFERENCES:

Marlow, W. and R. L. Tanner, "Diffusion Sampling Method for Ambient Aerosol Size Discrimination with Chemical Composition Determination," *Anal. Chem., 48*, 1999, November 1976.

Tanner, R. L. and W. H. Marlow, "Size Discrimination and Chemical Composition of Ambient Airborne Sulfate Particles by Diffusion Sampling," *Atmos. Environ.*, 1977 (in press).

TASK 6: Pollutant Transformation

SUB-TASK: 6. Numerical Modeling Homogeneous, Gas Phase Kinetics of NO_x, SO_2 and Hydrocarbons

CONTACT: R. F. Adamowicz

OBJECTIVE: Development of a mechanistic and simulative atmospheric kinetic model incorporating NO_x-O_3-hydrocarbon chemistry and generalized oxy-radical-SO_2 sulfate production.

RESEARCH ACTIVITIES: A preliminary kinetic model which describes the homogeneous gas phase chemistry of important atmospheric pollutants such as SO_2, hydrocarbons, oxides of nitrogen, carbon monoxide, ozone and other oxidants has been developed for use in generating, testing and delineating the validity of highly parameterized kinetic schemes needed for urban and regional scale pollution transport and transformation models. The kinetic model incorporates 41 mechanistic and simulative reactions in 28 chemical species and includes 5 oxy-radical-SO_2 reactions leading to sulfate aerosol production. A numerical computer model, PI RACKS: a Program for Integrating Rates of Atmospheric Chemical Kinetic Systems, has also been developed that defines the differential rates through a matrix representation of the chemical kinetic mechanism. The matrix representation facilitates rapid testing and modifications of the mechanism without laborious recording problems. The diurnal variation of the rates of the photolytic reactions as a function of the latitude, longitude, month, day and year of the simulated air parcel is also included in the numerical model.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Adamowicz, R., "PIRACKS: A Program for Integrating the Rates of Atmospheric Chemical Kinetic Systems," 1977, in preparation.

TASK 7: Surface Removal Processes

SUB-TASK: 1. Dry Deposition Studies

CONTACT: B. B. Hicks and M. L. Wesely

OBJECTIVE: Parameterization of the atmospheric and surface properties that affect the gaseous and particulate deposition rates at the surface of the earth.

RESEARCH ACTIVITIES: The properties of the atmosphere and the underlying surface that affect the vertical transport of trace gases and small particles in the atmospheric surface layer have been investigated. Parameterization schemes, based on previous and ongoing research, have been developed to describe the vertical fluxes of trace gases for a wide range of atmospheric conditions, over various types of surfaces. Work on sulfur dioxide has been emphasized. During 1976, preliminary measurements of the deposition of sulfur dioxide and small particles took place over winter grass. Also, in the summer, ozone fluxes were measured over corn. Results of analyses indicate that particle fluxes are larger than usually assumed over vegetated surfaces, and that several surface properties, as well as total dose of ozone, appear to control the reactivity of ozone with the corn leaf surfaces.

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATION: EPA

REFERENCES:

Hess, G. D. and B. B. Hicks, "The Influence of Surface Effects on Pollutant Deposition Rates over the Great Lakes," *Proceedings of the Second Federal Conference on the Great Lakes*, 338-347, 1976.

Hicks, B. B. and P. S. Liss, "Transfer of SO_2 and Other Reactive Gases Across the Air-Sea Interface," *Tellus, 28*, 348-354, 1976.

Wesely, M. L., B. B. Hicks, W. P. Dannevik, S. Frisella and R. B. Husar, "An Eddy-Correlation Measurement of Particulate Deposition from the Atmosphere," *Atmos. Environ., 11*, 561, 1977.

Wesely, M. L. and B. B. Hicks, "A Review of Some Factors that Affect the Deposition Rates of Sulfur Dioxide and Similar Gases on Vegetation," *JAPCA, 27*, 1110-1116, 1977.

Wesely, M. L., "Relationships Between Dry Deposition Rates and Concentrations at Heights of 50-200 m," presented at the 70th Annual AIChE Meeting, New York, N.Y., November 1977.

Hicks, B. B., "On the Parameterization of Aerosol Fluxes to the Great Lakes," *J. for Great Lakes Research* (in press), 1978.

Hicks, B. B., "Some Micrometeorological Methods for Measuring Dry Deposition Rates," presented at the 70th Annual AIChE Meeting, New York, N. Y., November 1977.

TASK 8: Pollutants and Precipitation

SUB-TASK: 1. MAP3S Precipitation Chemistry Network

CONTACT: M. Terry Dana and J. M. Hales

OBJECTIVE: Establishment of a valid precipitation chemistry data base for use in regional model development.

RESEARCH ACTIVITIES: A limited northeast regional precipitation chemistry sampling network (cf. Fig. 2) has been put into operation during the past year. Special samplers have been designed and constructed for this network, and these are being operated in conjunction with conventional (HASL) samplers for comparison purposes. Samples are obtained by individual network operators on an event basis and shipped to Battelle-Northwest for chemical analysis. Species analyzed include H^+, conductivity, $SO_3^=$, $SO_4^=$, NH_4^+, NO_2^-, NO_3^-, Cl^-, PO_4^{3-}, Na^+, Mg^{++}, Al^{3+}, K^+, and Ca^{++}. Conventional techniques of automated colorimetery and atomic absorption spectrophotometry are combined with ion chromatography to perform these analyses.

Monthly computer printouts of concentration and field data are being issued (beginning with January 1977) to interested parties. The data are also stored on cards and will be compiled into annual or semi-annual reports for wider distribution.

The basic intent of this project is to provide the high-quality precipitation chemistry data required for regional assessment of fossil-fuel impact. The duration of this network will be about three years, and it is viewed as a forerunner for an extensive national precipitation chemistry network which is anticipated for future deployment. Techniques and methodologies developed from the present, modest network will constitute a useful information base for design of this more ambitious program.

REPORTING ORGANIZATION: Battelle, Pacific Northwest Laboratories

COOPERATING ORGANIZATIONS: Collection Sites

1. Whiteface Mountain Field Station
   Atmospheric Sciences Research Center
   State University of New York at Albany
   Ray Falconer and Gerald Wolfe

2. Department of Ecology and Systematics
Cornell University
Ithaca, NY
Gene Likens and Tom Butler

3. Department of Meteorology
Pennsylvania State University
University Park
Rosa de Pena and Van C. Bowersox

4. Department of Environmental Sciences
University of Virginia
Charlottesville
James N. Galloway and Jesse Parker

NOAA, Air Resources Laboratory (Willaim Elliot)
EML (Herbert Volchok)

REFERENCES:

Hales, J. M., M. T. Dana and D. W. Glover, "Sampling for Volatile Trace Constituents in Natural Precipitation," submitted to *Atmos. Environ.*, 1977.

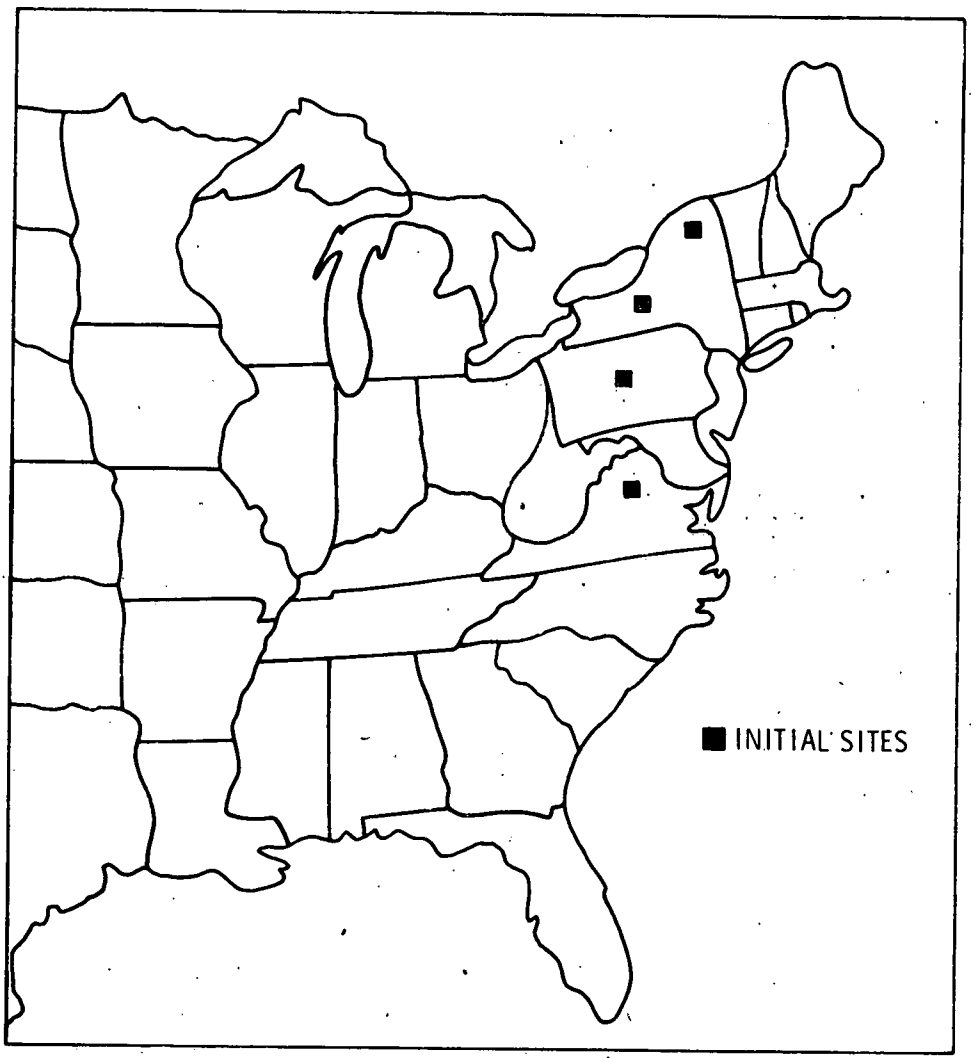

FIGURE 2. MAP3S Precipitation Chemistry Network.

TASK 8: Pollutants and Precipitation

SUB-TASK: 2. Precipitation Sampling

CONTACT: G. S. Raynor, BNL

OBJECTIVE: Document constituents and characteristics of precipitation on Long Island and relate these to pertinent meteorological factors and pollutant source distribution. Separate effects of rainout and washout.

RESEARCH ACTIVITIES: The precipitation sampler was placed in service June 1, 1976. Over 500 hourly precipitation samples have been collected through May 1977 and have been analyzed for pH, conductivity, nitrates, ammonia, sulfates, sodium and chloride. Meteorological data have also been recorded for each sample. Preliminary analyses of data have been accomplished. An Illinois State Water Survey raindrop size sampler was installed in early December 1976.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: ISWS

REFERENCES:

Raynor, G. S., "Meteorological and Chemical Relationships from Sequential Precipitation Samples," BNL Report #22879, 1977.

TASK 8: Pollutants and Precipitation

SUB-TASK: 3. METROMEX Network Chemistry Studies

CONTACT: R. G. Semonin, ISWS

OBJECTIVE: To investigate the temporal and spatial variability of dry and wet deposition of elements and compounds observed in proximity to the St. Louis urban-industrial metropolitan area. The goal of this task is to achieve parameterization for numerical models through understanding the physical processes.

RESEARCH ACTIVITIES: The network rainwater samples acquired during the 1972-1975 field activities have been chemically analyzed for a number of trace metals, pH, conductivity, and SO_4. The number of analyses undertaken is dependent on the amount and areal coverage of precipitation so the data set is not complete for all experiments. Contoured maps of each case are nearly complete, and statistical analyses are being undertaken to characterize the precipitation chemistry climatology of the area.

REPORTING ORGANIZATION: Illinois State Water Survey

COOPERATING ORGANIZATIONS: State of Illinois; NSF/RANN; EPA; ANL; PNL; University of Chicago; University of Wyoming; SRI, International; NOAA.

REFERENCES:

"METROMEX Update," *Bull. Amer. Meteoro. Soc., 57*(3), 304-308, 1976. Contains references to pertinent results through 1974.

Semonin, R. G., et al., *Study of Air Pollution Scavenging, Fifteenth Progress Report*, Illinois State Water Survey Report COO-1199-58, 1977.

TASK 8: Pollutants and Precipitation .

SUB-TASK: 4. Study of the Precipitation pH in Illinois

CONTACT: Gary J. Stensland, ISWS

OBJECTIVE: Calculation of pH from the detailed chemical analysis available for 35 precipitation samples collected in 1954 and comparison to recent data. Goal is to develop techniques for pH determinations of MAP3S precipitation samples collected in proximity to Chicago.

RESEARCH ACTIVITIES: Researchers measuring the chemistry of precipitation have found that an ion charge balance for major cations and anions can provide a reasonable estimate of the pH of the solution. As a prelude to MAP3S precipitation sampling in proximity to Chicago, the efficacy of this method of pH determination was studied. This approach was applied to six months of event (or sequential) wet only samples for 1954 and one month of event samples for 1960, for which pH measurements are not available. The reported alkalinity data provide an independent estimate of the pH which agrees very well with the ion balance pH. A comparison is made between these early pH estimates and the measured pH values for 1975-76. The recent weekly and event samples are obtained on the roof of the Water Survey building, seven miles northeast of the 1954, 1960 site in Champaign-Urbana (a midwestern town of 100,000 population and little industry).

The arithmetic average pH is 5.4 for the 1954 samples and 4.3 for the 1975-76 weekly samples. Another indication of the decreasing pH trend at Champaign-Urbana is that of the 36 samples for 1954, 50% have estimated pH values greater than 6.0 while samples with pH greater than 6.0 have been observed very infrequently in the 1975-76 data. Additional field measurements are now in progress to provide explanations for the pH decrease.

REPORTING ORGANIZATION: Illinois State Water Survey

COOPERATING ORGANIZATIONS: State of Illinois; NSF/RANN; EPA; ANL; PNL; University of Chicago, University of Wyoming; SRI, International; NOAA.

REFERENCES:

Stensland, G. J., "Precipitation pH Decrease Since 1954 at Champaign-Urbana, Illinois," in *Study of Air Pollution Scavenging, Fifteenth Progress Report*, Illinois State Water Survey Report COO-1199-58, 1977.

TASK 8: Pollutants and Precipitation

SUB-TASK: 5. Chemical Tracer Scavenging Study

CONTACT: R. G. Semonin, ISWS

OBJECTIVE: Through the use of unique chemical tracers, to obtain scavenging efficiency of convective storms. These efficiencies will be used as guidance for numerical parameterization of sulfur scavenging by precipitation.

RESEARCH ACTIVITIES: Both aircraft and surface releases of tracers indium, lithium, and cesium were accomplished during the 1972-1975 field projects. The tracer lithium was released by acetone solution combustion while indium was released both by pyrotechnics and acetone solution aerosol generators. The tracer cesium was released by pyrotechnics only. The preliminary results indicate precipitation removal efficiencies ranging between 10% and > 100%. The correction of the rain concentrations for background contamination is underway with corresponding alterations of efficiency.

REPORTING ORGANIZATION: Illinois State Water Survey

COOPERATING ORGANIZATIONS: State of Illinois; NSF/RANN; EPA; ANL; PNL; University of Chicago; University of Wyoming; SRI, International; NOAA.

REFERENCES:

"METROMEX Update," *Bull. Amer. Meteoro. Soc.*, 57(3), 304-308, 1976. Contains references to pertinent results through 1974.

Semonin, R. G., et al., *Study of Air Pollution Scavenging, Fifteenth Progress Report*, Illinois State Water Survey Report COO-1199-58, 1977.

TASK 8: Pollutants and Precipitation

SUB-TASK: 6. Re-Analysis of ANL Precipitation Scavenging Data

CONTACT: B. B. Hicks, ANL

OBJECTIVE: To re-evaluate the results of an extensive investigation of concentrations of natural radioactivity attached to background aerosol, with the intent of deducing precipitation scavenging rates appropriate for application in the case of submicron sulfate particles.

RESEARCH ACTIVITIES: A set of radon daughter concentrations, measured in rain collected during several periods of extensive rain at Argonne in 1966, was previously analyzed employing overly simple conceptual models of the processes involved. The data obtained have been analyzed again, in order to derive better estimates of the rates at which background aerosol particles are scavenged by raining clouds typical of the MAP3S region.

REPORTING ORGANIZATION: Argonne National Laboratory

REFERENCES:

Hicks, B. B., "An Evaluation of Precipitation Scavenging Rates of Background Aerosol," *J. Appl. Meteorol.*, 1978 (in press).

TASK 8: Pollutants and Precipitation

SUB-TASK: 7. Precipitation Chemistry Modeling

CONTACT: R. F. Adamowicz, BNL

OBJECTIVE: Develop a model to assess the significance of the chemical and meteorological parameters encompasing the reversible washout of trace gases (SO_2, NH_3 and CO_2) from the atmosphere by rain and the aqueous phase production of sulfates.

RESEARCH ACTIVITIES: A model has been developed to describe the washout of trace atmospheric gases and the production of acids in rain. The model is applied to washout of sulfur dioxide, carbon dioxide and ammonia and incorporates reversible mass transfer of the trace gases, all possible ionic equilibria of the compounds in solution and catalyzed oxidation of the dissolved sulfur species to sulfates.

The significance of ammonia and carbon dioxide on the raindrops capacity for sulfur and on sulfate production based solely on bisulfate oxidation were explored in detail. The influence of raindrop size, rainfall intensity, cloud-base height, the presence of oxidation catalyzing compounds in the atmosphere and the initial composition of the raindrops as they enter the polluted atmospheric layer on the detailed chemical composition of rain at ground level and the time scale for gaseous sulfur dioxide removal has been evaluated.

Illustrative model simulations suggest that the chemical composition of rain is, in general, mass-transfer rate limited. Carbon dioxide was found to have little effect on the concentration transients or the approach to equilibrium composition of raindrops as they fall through the mixed layer. Ammonia, however, considerably increases rain's capacity for sulfur and causes the chemical composition of even small droplets (light rainfalls) to be mass-transfer rate limited. In addition, the effect of a background non-volatile base (such as NaOH) on the transient composition of rain was found to be quite different than the effect of a volatile base (NH_3), giving rise to a step-function behavior of the transient pH and

aqueous sulfur dioxide concentration. The presence of a non-volatile base in the atmosphere may cause occurrence of a bimodal pH distribution in raindrop size spectra.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Hill, F. B., and R. F. Adamowicz, "A Model for Rain Composition and the Washout of Sulfur Dioxide," *Atmos. Environ.*, 1977 (in press).

Adamowicz, R. F. and F. B. Hill, "A Model for the Reversible Washout of Sulfur Dioxide, Ammonia, and Carbon Dioxide from a Polluted Atmosphere and the Production of Sulfate in Raindrops," presented at 70th AIChE Annual Meeting, New York, November 1977 (available as BNL Report 22576).

TASK 8: Pollutants and Precipitation

SUB-TASK: 8. Precipitation Scavenging

CONTACT: B. C. Scott and J. M. Hales, PNL

OBJECTIVE: Determination of wet removal parameters necessary for formulation of reliable regional models of pollution behavior.

RESEARCH ACTIVITIES: Preliminary aircraft and surface measurements were made at the Muskegon field site during the late winter of 1977. These included airborne measurement of gaseous and particulate pollutants in the storm systems, collection and chemical analysis of supercooled cloud water, and physical and chemical analysis of precipitation at ground level. Because of the unexpected loss of an engine on the research aircraft, these measurements were deferred until later than the desired period, and thus the more ideal lake effect storms were not encountered. Nevertheless, some valuable information has been obtained from these measurements.

During August 1977 a tracer characterization flight series was performed at Muskegon, which provided large amounts of significant data regarding the performance of the DC-3 acetone tracer-generation system. This system will be employed for scavenging studies during the coming year.

At the present time activities are underway to conduct an extensive lake-effect storm study during the December-January period. Cooperative research projects with NSF-funded groups (ISWS and University of Chicago) have progressed as planned, and their facilities are currently onsite and operating. These include the CHILL Doppler-radar, which has been positioned to the north of Muskegon, and the NCAR Queenaire aircraft, which has been instrumented for cloud physics measurements by the University of Chicago.

REPORTING ORGANIZATION: Battelle, Pacific Northwest Laboratories

COOPERATING ORGANIZATION: University of Michigan, ISWS, University of Chicago, NCAR.

REFERENCES:

Hales, J. M. et al., "Pacific Northwest Laboratory Annual Report for 1976 to the ERDA Assistant Administrator for Environment and Safety," BNWL-2100 Pt. 3, 232 p., August 1977.

TASK 9: Weather and Climate Modification

SUB-TASK: 1. Turbidity Experimental Network

CONTACT: M. L. Wesely, ANL

OBJECTIVE: To determine the extent of regional-scale episodes of increased haze in the northeastern United States and to assess the associated changes in solar radiation.

RESEARCH ACTIVITIES: Analysis of atmospheric turbidity at Argonne has suggested that most of the haze in summer does not originate locally, but is associated with occassional regional-scale events. Further measurements of turbidity, by use of a simple inexpensive pyranometer tested successfully for a month in an arc downwind of St. Louis, also seemed to show that local sources of particulate matter had a small effect relative to regional-scale transport of aerosols into the area. To examine the variations of atmospheric turbidity temporally and spatially in the MAP3S region, a network of ten stations for the pyranometers has been established. The sites were chosen on the basis of an objective analysis of past turbidity data. The pyranometer, a silicon-cell device, has been extensively compared with more standard thermopile pyranometers, so that the data can be interpreted more easily.

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATIONS: The present sites have been supplied by: BNL, NWS, Miami University of Ohio, ORNL, Missouri Department of Natural Resources, ERT, Kansas State University at Manhattan, University of Guelph in Ontario, University of Michigan at Pellston Station, Pennsylvania State University at University Park, and the University of Virginia at Charlottesville.

REFERENCES:

Wesely, M. L. and R. C. Lipshutz, "An Experimental Study of the Effects of Aerosols on Diffuse and Direct Radiation Received during the Summer Near Chicago," *Atmos. Environ.*, *10*, 981-987, 1976.

Wesely, M. L., "Measurements of Atmospheric Turbidity in an Arc Downwind of St. Louis," ANL-75-60 Part IV, Radiological and Environmental Research Division Annual Report, January-December 1975, pp. 22-30, 1976.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 1. Development of Numerical Schemes

CONTACT: C. M. Sheih

OBJECTIVE: To develop improved schemes for solving finite-difference equations of diffusion and for parameterizing subgrid-scale pollutant clouds.

RESEARCH ACTIVITIES:

1. A puff-on-cell model for computing pollutant transport and diffusion has been developed; this minimizes the pseudo-diffusion which arises in numerical solutions of the finite-difference equations of turbulent diffusion and transport.
2. A Lagrangian puff diffusion model with wind shear and dynamic plume rise has been developed for use in predicting pollutant concentrations in unsteady or non-uniform flow conditions and for use in parameterizing subgrid-scale pollutant clouds in grid models.

REPORTING ORGANIZATION: Argonne National Laboratory

REFERENCES:

Sheih, C. M., "A Puff-Grid Model for Predicting Pollutant Transport Over an Urban Area," *J. Air Poll. Control Assoc.*, *27*, 184-185, 1977.

Sheih, C. M., "Mathematical Modeling of Particle Coagulation and Transport Downstream of an Urban Area Source," *Atmos. Environ.* (in press), 1978.

Sheih, C. M., "A Puff-on-Cell Model for Computing Pollutant Transport and Diffusion," *J. Appl. Meteorol.* (in press), 1978.

Sheih, C. M., "On the Relative Importance of Single-Particle and Relative Diffusion for Plume Dispersion," submitted to *Tellus*, 1977.

Sheih, C. M., "A Puff Pollutant Dispersion Model with Wind Shear and Dynamic Plume Rise," submitted to *Atmos. Environ.*, 1977.

Yamada, T., "A Numerical Experiment on Pollutant Dispersion in a Horizontally-homogeneous Atmospheric Boundary Layer," *Atmos. Environ.* (in press), 1978.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 2. Model Development

CONTACT: D. C. Powell, L. L. Wendell, and W. E. Davis, PNL

OBJECTIVE: To develop segmented computer models which will simulate the behavior of the atmosphere and its contaminants from source to receptor in the region of interest. The models should be capable of describing transport, dispersion, chemical transformation, aerosol behavior, dry deposition and precipitation scavenging with enough realism to produce reliable and reasonably economical assessments of power production pollutants.

RESEARCH ACTIVITIES: The approach of this work has been to construct a model containing the necessary components in simple form and to use this model as a vehicle for improvement. One version of the model as it has been developed to this point treats the transport, dispersion, transformation and removal processes in a Lagrangian sense. Plumes from one or more point sources (power plants) are broken into segments containing the emission for a 1-hour time period. The material in these segments are transported and dispersed through a single layer by the average winds in the layer. The winds are obtained by a space and time interpolation of the 12-hourly radiosonde data produced by the National Weather Service. In this version of the model the material (initially SO_2) in each plume segment is chemically transformed in a linear fashion as a function of time and is treated as a mixture of two separate constituents (SO_2 and sulfate particulate) which have different properties in the wet and dry removal processes. The dry removal is dependent on the mixing layer depth and specified deposition velocities for the two constituents. Wet removal is dependent on a bulk dropsize, precipitation rate and specified collection efficiencies for the two constituents. The model is designed to accept hourly precipitation rates averaged in each square of the sampling grid.

Another version of the model has been developed to treat the transport in eight layers using isentropic considerations to simulate vertical motions in a more realistic manner in the vicinity of frontal storms.

REPORTING ORGANIZATION: Battelle, Pacific Northwest Laboratories

COOPERATING ORGANIZATIONS: ANL, ARL, BNL

REFERENCES:

Davis, W. E. and L. L. Wendell, "Some Effects of Isentropic Vertical Motion Simulation in a Regional Scale Quasi-Lagrangian Air Quality Model," in *Pacific Northwest Laboratory Annual Report for 1976 to the ERDA Assistant Administrator for Environment and Safety*, BNWL-2100, Pt. 3, 232 p., August 1977.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 3. Model Testing and Application

CONTACT: L. L. Wendell, T. D. Fox and D. J. McNaughton, PNL

OBJECTIVE: To test separate model components as well as the models as a whole for both accuracy and sensitivity. Accuracy of the models is important for providing realistic assessments and sensitivity is important from the standpoint of providing long-term assessments within reasonable economic bounds.

RESEARCH ACTIVITIES: In an effort to examine the sensitivity of the model to the real-time variability in precipitation, a computer technique was developed to utilize hourly precipitation data measured at about 800 randomly spaced locations in the Northeast United States and produce hourly gridded maps of the precipitation distribution to be used for precipitation scavenging in model calculations. One month of data was produced for model testing.

A test of model sensitivity to precipitation scavenging by average vs. real-time precipitation was conducted for the one month period of the rain data. The major conclusions from this preliminary testing were that, for the parameterizations used, the average precipitation removed almost twice as much material, over the whole grid, as did the real-time precipitation case for the same time period. The deposition patterns produced by the use of the real-time precipitation data were quite different from those produced by use of average precipitation data and would not have been reasonably approximated by a factor of two reduction in the collection efficiency for the average precipitation case.

A sort merge technique has been devised to put the hourly precipitation data available at Ashville, N. C. into a form suitable for producing hourly gridded data for periods of one or more years. This program is currently in the checkout phase and will undergo further testing.

REPORTING ORGANIZATION: Battelle-Pacific Northwest Laboratories

COOPERATING ORGANIZATIONS: BNL, ARL, ANL

REFERENCES:

Wendell, L. L., D. C. Powell and D. J. McNaughton, "A Multisource Comparison of the Effects of Real-Time vs. Time-Averaged Precipitation Data on SO_2 and Sulfate Particulate Removal in a Regional Air Quality Model," in *Preprint Volume of the Joint Conference on Applications of Air Pollution Meteorology*, Salt Lake City, Utah, November 1977.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 4. Modeling of Long-Range Transport

CONTACT: Jerome L. Heffter, NOAA-ARL

OBJECTIVE: To modify and further develop the ARL transport and dispersion models for use in MAP3S related programs.

RESEARCH ACTIVITIES: The ARL regional-continental scale model now includes vertical temperature profile and wind shear data to determine vertical mixing depths. A mesoscale model is being developed with finite difference calculations in the vertical which can include the effects of dry and wet deposition.

REPORTING ORGANIZATION: NOAA-Air Resources Laboratory

REFERENCES:

Heffter, J. L and A. D. Taylor, "Trajectory Model. Part I. 'A Regional-Continental Scale Transport, Diffusion and Deposition Model'," NOAA Technical Memo ERL ARL-50, 28 p., 1975.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 5. Application of a Lagrangian Statistical Trajectory Model

CONTACT: C. M. Sheih, ANL

OBJECTIVE: To simulate sulfur dioxide and sulfate dispersion over the northeastern United States.

RESEARCH ACTIVITIES: A model of atmospheric sulfur pollution for the region of interest to MAP3S has been developed. The model approximates the long term average plume from each large pollutant source by a series of Lagrangian puffs in which the horizontal distribution is assumed to be Gaussian. To construct the puffs, a simulated tracer particle is released twice a day and its location is computed at three hour intervals by use of observed wind velocities. The location of the center of each puff at certain times after release is computed by averaging the coordinates of all the particles at the same time after release, and the standard deviations of these coordinates with respect to the puff center are used to define the puff size. The vertical distribution of material in each puff is computed by numerical integration of a system of two equations which describe the budgets of sulfur dioxide and sulfate, with consideration of inversion height, surface deposition, effective stack height, and chemical transformation. These four factors have been varied in a series of sensitivity tests for the model. The final concentrations of sulfur dioxide and sulfate at a point of interest are obtained by summing the contributions of all the puffs to that point. In the present simulation, pollutant sources of sulfur dioxide originating from 53 major power plants in the northeastern United States are considered, and maps of the predicted sulfur dioxide and sulfate concentrations at 2 m height and of the dry deposition of sulfur have been obtained.

REPORTING ORGANIZATION: Argonne National Laboratory

REFERENCES:

Sheih, C. M., "Application of a Statistical Trajectory Model to the Simulation of Sulfur Pollution over the Northeastern United States," *Atmos. Environ.*, *11*, 173-178, 1977.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 6. Regional Three-Dimensional Eulerian Diffusion-Advection Model with Nonlinear Chemical Reactions

CONTACT: R. E. Meyers, R. T. Cederwall and J. Storch, BNL

OBJECTIVE:

A. To develop a three-dimensional regional Eulerian-grid transport, diffusion and chemical reaction (air quality) model for MAP3S.

B. To develop methods for examining and to evaluate the importance of including turbulence mixing in air quality models.

C. To establish a meteorological computer data link between National Weather Service, Suitland, MD and Brookhaven National Laboratory to be able to make near real-time air quality/meteorological calculations.

RESEARCH ACTIVITIES:

A. A review is underway of candidate numerical approaches. Numerous techniques have already been investigated. An improved finite moment method of incorporating diffusion has been developed. A three-dimensional particle in cell model has been developed to run in a height normalized non-orthogonal coordinate system over complex terrain. Assessments of power plant health impacts have been made using the existing BNL trajectory-numerical model.

B. A turbulence-chemistry plume model has been developed to handle nonlinear chemical reactions using probability methods. A method for calculating entrainment of chemicals into plumes has been developed using intermittency concepts.

C. A Suitland to BNL data system has been designed. A minicomputer and basic hardware and some software components have been ordered. Software system development has begun.

D. The framework for an objective-diagnostic model has been developed using the method of optimal statistical interpolation and variational analysis. The model includes complex terrain and meteorological sounding data. A method has been developed for incorpor-

ating wind and density profiles into the layered model which extends from the terrain to the tropopause.

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: NOAA-TDL, White Sands Missile Range (ASL)

REFERENCES:

Meyers, R. E., R. T. Cederwall, W. D. Ohmstede and W. aufmKampe, "Transport and Diffusion Using a Diagnostic Mesoscale Model Employing Mass and Total Energy Conservation Constraints," *Preprints of the Third Symposium on Atmospheric Turbulence, Diffusion and Air Quality*, American Meteorological Society, Raleigh, N. C., October 1976.

Lopazo, C., "A Probabilistic Approach to the Turbulent Mixing of Reactive Scalars," *Preprints of the Third Symposium on Atmospheric Turbulence, Diffusion and Air Quality*, American Meteorological Society, Raleigh, N. C., October 1976.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 7. Support of Experimental Programs

CONTACT: L. L. Wendell and D. C. Powell

OBJECTIVE: To put the models, where possible, to use in aiding the planning of experiments to be conducted to provide insight and information necessary for the simulation effort.

RESEARCH ACTIVITIES: Special computer output to microfilm (COM) graphics programs have been developed to display time sequences of plume positions. Plots of this type were used to aid in the interpretation of the "finger-print" samples in urban plumes, by showing whether or not the samples were taken in unique plumes or a combination of plumes from other locations.

An animated version of this program was devised to allow a dramatic visualization of plume behavior and provide some insight into where to look for plumes from a stack under various evolving synoptic weather patterns.

In an effort to get a better approximation of the $SO_2 \rightarrow SO_4^{=}$ transformation, a simple formulation was devised to use the aircraft measurements of the St. Louis plume. Measurements of the SO_2 and total sulfur downwind of the city were used to obtain estimates of transformation parameters.

REPORTING ORGANIZATION: Battelle, Pacific Northwest Laboratories

COOPERATING ORGANIZATIONS: BNL, ARL, ANL

REFERENCES:

Alkezweeny, A. J. and D. C. Powell, "Estimation of Transformation Rate of SO_2 to SO_4 From Atmospheric Concentration Data," *Atmos. Environ., 11*, 179, 1977.

Hales, J. M. et al., "Pacific Northwest Laboratory Annual Report for 1976 to the ERDA Assistant Administrator for Environment and Safety," BNWL-2100 Pt. 3, 232 p., August 1977.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 8. Acquisition, Archiving, and Dissemination of Experimental Data Generated by MAP3S and Related Programs.

CONTACT: C. Benkovitz, BNL

OBJECTIVE: Acquisition, archiving and dissemination of experimental data generated by MAP3S and related programs.

RESEARCH ACTIVITIES: The development of a computerized, general purpose index of MAP3S experiment has been started. Reporting forms have been sent to MAP3S participants and a prototype computerized data base is being implemented.

Establishment of standard format for computer comparable data flow to/from BNL central repository will be based on the work of two other ERDA-sponsored programs:

1. The Inter-Laboratory Working Group for Data Exchange and its work in developing what is currently the proposed ANSI standard.
2. The Light Water Reactor Environmental Effects Program in sponsoring the development of the computer software needed to implement such a standard at its associated DOE laboratories.

Contact has been established with Environmental Research and Technology, Inc. (ERT), contractors of the SURE (Sulfate Regional Experiment) program for the Electrical Power Research Institute (EPRI). Initial procedures for exchange of experimental data between MAP3S and SURE have been tentatively worked out.

REPORTING ORGANIZATION: Brookhaven National Laboratory

REFERENCES:

Austin, D. L. and D. Merrill, "ERDA Interlaboratory Working Group for Data Exchange (IWGDE)," Annual Report for FY-1976, LBL-5329, Lawrence Berkeley Laboratory, September 1976.

ANSI Subcommittee X3L5, Draft Proposal, "American National Standard Specifications for an Information Interchange Data Descriptive File," Working Paper ANSI/X3L5/589F, Am. Natl. Standards Institute, Feb. 1977.

Benkovitz, C. M., "Facilitating Data Interchange Within ERDA," BNL-22595, Brookhaven National Laboratory, April 1977. Presented at VIM-26 Meeting, Minneapolis, Minn., Apr. 4-7, 1977.

SECTION 2

PLANNED RESEARCH ACTIVITIES

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TASK 1: Power Production Emissions

SUB-TASK: 1. Source Characterization

CONTACT: R. N. Dietz, BNL

OBJECTIVE: Verify sampling techniques, characterize emissions, and determine the relevant combustion and control parameters affecting these emissions.

RESEARCH PLAN: The principal sampling techniques, including the EPA Method 6 isopropyl alcohol bubbler approach and the BNL and EPA controlled condensation methods, will be evaluated both in the laboratory and at an oil-fired power plant. Several sampling efforts with the concurrent participation of BNL and EPA will further validate techniques.

Detailed sampling experiments at controlled and uncontrolled power plant units will be performed with different conditions of power level, excess furnace oxygen, fuel sulfur content, precipitator operating level, additives, and ambient humidity ranges. Effects on emissions of sulfuric acid, particulate sulfate, total particulates, principal metals and carbon, and gaseous nitrogen oxides will be determined. Correlation of the emissions as a function of significant parameters will be attempted.

The next stage will require similar sampling at different power plants using different fuels and burner designs and at industrial boilers, apartment furnaces, and home heating units. Projected impact of each type of combustion sources on the overall pollution levels in specified regions will be assessed.

FIELD LOCATION: BNL and nearby LILCO plant

FIELD EXPERIMENT TIMETABLE: Continuing

REPORTING ORGANIZATION: Brookhaven National Laboratory

COOPERATING ORGANIZATIONS: EPA, EPRI, LILCO

PROJECT DURATION: Continuing

REFERENCES:

Dietz, R. N. and R. F. Wieser, "Sulfate Emissions from Fossil Fueled Combustion Sources," BNL Semi-Annual Report No. 4, February 1977.

TASK 1: Power Production Emissions

SUB-TASK: 2. Emissions Inventory Compilation

CONTACT: C. M. Benkovitz, BNL

OBJECTIVE: Compile best estimate emissions inventory.

RESEARCH PLAN: Continuation of activities described in the Brief Project Report Section. Early user access to computerized data bases will be encouraged by development of appropriate user documentation. Updates of NEDS data (first update, December 1976 recently received) will be incorporated into the existing data bases.

Initial studies of available data will concentrate on correcting gross errors and omissions. Examples of this type of error are point sources with missing or erroneous locations. More detailed quality assessment of the data will be undertaken as time and manpower allow.

Methodologies for reformatting and handling the data will be generalized and combined whenever possible and made available to users. Auxiliary data will also be formatted and made available in a suitable way.

DEVELOPMENT STATUS: Data from EPA and FPC have been received and initial inventories compiled.

PLANNED AVAILABILITY: Data should be available for model studies in late 1977.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

TASK 2: Nonpower Production Emissions

SUB-TASK: 1. Nonenergy Related Point Source

CONTACT: L. Newman and J. Forrest, BNL

OBJECTIVE: Further studies on nature of the oxidation of SO_2 in non-energy related point sources.

RESEARCH PLAN: Study the source emission of sulfur dioxide and sulfate from smelter, refinery and steel mill operations and the conversion rate of sulfur dioxide in the plumes thereof. The objective is to obtain a basis to assess the contribution of these operations to the sulfur levels in the MAP3S region. The MAP3S-designated BNL operated airplane will be deployed to sample the plumes. Typical flight patterns will consist of sampling at 1, 3, 10 and 30 miles downwind of the source. The measurements will center upon utilization of the BNL filter pack to obtain integrated samples of sulfate and sulfur dioxide. Concurrent gaseous and aerosol will be made. Data will be obtained during day and night time operations and high and low temperature and humidity regimes. The importance of homogeneous and heterogeneous mechanisms will be assessed.

FIELD LOCATION: Selected power plants in the northeast.

FIELD EXPERIMENT TIMETABLE: Spring and summer 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Two years

REFERENCES:

Newman, L., J. Forrest and B. Manowitz, "The Application of an Isotopic Ratio Technique to a Study of the Atmospheric Oxidation of Sulfur Dioxide in the Plume from an Oil-Fired Power Plant," *Atmos. Environ.*, *9*, 959, 1975.

Newman, L., J. Forrest and B. Manowitz, "The Application of an Isotopic Ratio Technique to a Study of the Atmospheric Oxidation of Sulfur Dioxide in the Plume from a Coal-Fired Power Plant," *Atmos. Environ.*, *9*, 969, 1975.

Romano, J., J. H. Klein, and L. Newman, "An Air Sampling System to Measure Power Plant Effluents Using a Lightweight Aircraft," *J. Environ. Systems*, *5*, 271, 1975.

Forrest, J. and L. Newman, "Further Studies of the Oxidation of Sulfur Dioxide in Coal-Fired Power Plant Plumes," *Atmos. Environ*, *11*, 465, 1977.

Forrest, J. and L. Newman, "Oxidation of Sulfur Dioxide in the Sudbury Smelter Plume," *Atmos. Environ.* (in press).

Schwartz, S. E. and L. Newman, "Processes Limiting the Oxidation of Sulfur Dioxide in Stack Plumes," *Environ. Sci. & Tech.*, 1977 (in press).

TASK 3: Pollutant Properties

SUB-TASK: 1. Development of Analytical Methods for Ground and Airborne Sampling

CONTACT: Roger L. Tanner, BNL

OBJECTIVE: Implementation of existing methods and development of new methods for the characterization of the chemical and physical nature of sulfate in airborne particles; development of improved analytical methodologies for other energy-related pollutants (nitrate, NH_3, etc.) in the atmospheric environment.

RESEARCH PLAN:

1. Validate extraction methodology for specific determination of H_2SO_4 and bisulfate.
2. Further investigate filter pack methods for NH_3 analysis.
3. Implement ion chromatographic method for simultaneous $SO_4^{=}$, NO_3^{-}, other.
4. Implement method for total mass measurement on quartz filter samples.
5. Investigate methods for nitrate speciation in airborne particles.
6. Evaluate interactions in nitrate with acid sulfate and of SO_2 with freshly collected aerosol on quartz filters.

FIELD LOCATION: BNL, Other Local

FIELD EXPERIMENT TIMETABLE: Continuing

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Tanner, R. L., R. W. Garber and L. Newman, "Speciation of Sulfate in Ambient Aerosols by Solvent Extraction with Flame Photometric Detection," presented at Environmental Chemistry, American Chemical Society Meeting, New Orleans, LA, March 20-25, 1977.

TASK 3: Pollutant Properties

SUB-TASK: 2. Development of Real-Time Instrumentation

CONTACT: Roger L. Tanner, BNL

OBJECTIVE: Develop method for analyzing total aerosol sulfur in real-time by flame photometric detection.

RESEARCH PLAN: Use Meloy 285 Sulfur Analyzer with appropriate pretreatment (particle filter, thermal treatment, diffusion denuding) to develop a method for real-time analysis of airborne particulate sulfur utilizing ambient aerosols, lab-generated aerosols and combinations thereof.

FIELD LOCATION: Aircraft, SURE Research Stations, BNL Tower

FIELD EXPERIMENT TIMETABLE: After January 1, 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: 2-3 Years

TASK 3: Pollutant Properties

SUB-TASK: 3. Aerosol Measurement

CONTACT: W. H. Marlow, BNL

OBJECTIVE: Development of aerosol instrumentation, associated analytical methods, and the theory of aerosol measurement.

RESEARCH PLAN:

1. The MAP3S-BNL airborne high volume aerosol sampler will be calibrated to assure known size separations of particles.
2. A high volume, ground-based aerosol sampler will be constructed to afford the capability of taking high time resolution filter samples.
3. Work in collaboration with HASL on the development of an analytical method for extraction of size distribution information from diverse aerosol measurement methods will be completed and reported.
4. A general treatment addressing the information content of aerosol measurements, including their stochastic component, and the determination of the aerosol size distribution from experimental data will be undertaken. The objective of this research will be the assessment of the degree of confidence that can be placed in size distribution determination and the specification of instrument design parameters to assure optimization of data acquisition.

DEVELOPMENT STATUS: Work is underway and should permit use of techniques in field studies by late 1977.

PLANNED AVAILABILITY: Techniques should be available in 1977 for use in BNL field studies.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Jaklevic, J. M., B. W. Loo, F. S. Goulding, "Dichotomous Virtual Impactors for Large Scale Monitoring of Airborne Particulate Matter," in *Fine Particles: Aerosols Generation, Measurement, Sampling and Analysis*, Benjamin Y. H. Liu (ed.), Academic Press, 1976.

Marple, V. A. and B. Y. H. Liu, "Characteristics of Laminar Jet Impactors," *Environ. Sci. & Tech., 8*, 648-654, July 1974.

Marlow, W. and R. L. Tanner, "Diffusion Sampling Method for Ambient Aerosol Size Discrimination with Chemical Composition Determination," *Anal. Chem., 48*, 1999, November 1976.

TASK 3: Pollutant Properties

SUB-TASK: 4. Measurement of Sulfate, Acid Sulfate, and Nitrate Content of Atmospheric Aerosols

CONTACT: P. Cunningham and R. Kumar, ANL

OBJECTIVE: Collect time- and size-resolved samples of atmospheric aerosols. Analyze the 0.3 to 1.0 micrometer diameter size fraction for its sulfate and nitrate content and for the extent of acidity of the sulfate.

RESEARCH PLAN: Lundgren-type impactors will be set up at up to five field sites for collecting four-hour samples of the ambient aerosol. Tentatively, every fifth sample from the Stage IV impacted samples will be analyzed by means of Fourier Transform Infra-Red Spectroscopy of a KBr pellet containing the sample. Neutral sulfate and nitrate will be determined quantitatively, with a qualitative assessment of the degree of acidity of the sulfate sample. The rest of the Stage IV samples, along with the Stage III samples (1.0 to 3.0 micrometer diameter particles) and the impactor after filters, will be retained as archive samples.

FIELD LOCATION: Site 1 - Pennsylvania State University, State College, PA

Site 2-5 - to be determined

FIELD EXPERIMENT TIMETABLE: Sampling at Site 1 to begin by January 31, 1977. Sites 2 and 3 to be operational by March 31, 1977. Schedule for Sites 4 and 5 yet to be determined.

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: Two to three years

REFERENCES:

Cunningham, P. T., S. A. Johnson and R. T. Yang, "Variations in Chemistry of Airborne Particulate Material with Particle Size and Time," *Environ. Sci. & Tech., 8*, p 131, 1974.

Cunningham, P. T., and S. A. Johnson, "Spectroscopic Observation of Acid Sulfate in Atmospheric Particulate Samples," *Science, 191*, p. 77, 1976.

TASK 3: Pollutant Properties

SUB-TASK: 5. Determination of Sulfur Speciation in Industrial Aerosols in an SO_2-Rich Environment.

CONTACT: Delbert J. Eatough, Brigham Young University

OBJECTIVE: The objective of this program is the development of analytical techniques for the identification of sulfur species (S(-II), S(IV), S(VI) and oxy sulfur acids) in industrial aerosols. Techniques to be used will include thermochemical analysis, ESCA, PIXE and SEM-EDAX techniques. In addition, a thermometric method has been developed for the identification of nitrate. These analytical techniques will be used for the study of the formation, transformation, and stability of S(IV) compounds in aerosols produced by smelters and fossil fuel burning stations.

RESEARCH PLAN: Phase I. Development of analytical techniques. Phase II. Study of S(IV) reactions in a coal-fired generating station, a copper smelter, and a steel mill plume. Phase III. Study of selected point sources to identify the effects of trace metal content, organic content, fuel type, SO_2 levels, acidity, humidity, and temperature on S(IV) chemistry in aerosol.

FIELD LOCATION: 4 Corners Power Plant, Garfield Smelter, USS Geneva Plant, several point sources to be selected in Phase III.

FIELD EXPERIMENT TIMETABLE: Coal-fired station plume February-March 1977 and possibly fall 1977. Copper smelter plume, February-July 1977. Steel mill plume, September-November 1977. Study of selected point sources, April-November 1978.

REPORTING ORGANIZATION: Brigham Young University

COOPERATING ORGANIZATIONS: Thermochemical Institute, Brigham Young University; Lawrence Livermore Laboratory, Livermore, CA.

PROJECT DURATION: 3 Years

REFERENCES:

Hansen, L. D., L. Whiting, D. J. Eatough, T. E. Jensen, and R. M. Izatt, "The Determination of Sulfur(IV) and Sulfate in Aerosols by Thermometric Methods," *Anal. Chem.*, *48*, 634, 1976.

Hansen, L. D., D. J. Eatough, N. F. Mangelson, T. E. Jensen, D. Cannon, T. J. Smith and D. E. Moore, "Sulfur Species and Heavy Metals in Particulates from a Copper Smelter," presented at the International Conference on Environmental Sensing and Assessment, Las Vegas, September 1975, pp. 23-3.

Eatough, D. J., L. D. Hansen, R. M. Izatt, and N. F. Mangelson, "Determination of Acidic and Basic Species in Particulates by Thermometric Titration Calorimetry," *Methods and Standards for Environmental Measurements*, NBS, September, 1976, in press.

Eatough, D. J., T. Major, J. Ryder, M. Hill, N. F. Mangelson, N. L. Eatough, L. D. Hansen, R. G. Meisenheimer, and J. W. Fischer, "The Formation and Stability of Sulfite Species in Aerosols," *Proceedings of the International Symposium on Sulfur in the Atmosphere*, Dubrovnik, Yugoslavia, September 1977.

TASK 4: Pollutant Distribution

SUB-TASK: 1. Objective Sensor Placement

CONTACT: J. D. Shannon, ANL

OBJECTIVE: Develop a scheme to model the spatial and temporal structure of atmospheric phenomena of interest to MAP3S and use that structure to locate sensors so that the data subsequently obtained have maximum value.

RESEARCH PLAN:

1. In collaboration with the related experimental team, develop a formal statement of the sensor-placement problem.
2. Obtain relevant observational data or model results.
3. Develop the correlation structure function describing the data.
4. Coordinate with field experimentalists in order to identify predetermined sensor locations.
5. Optimize locations of remaining sensors.

DEVELOPMENT STATUS: The technique has been applied to a ten-sensor regional turbidity network.

PLANNED AVAILABILITY: The technique can be applied to other sensor location problems with only minor alteration.

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: Through 1977

TASK 4: Pollutant Distribution

SUB-TASK: 2. Vertical Pollutant Distribution Experiment

CONTACT: R. Garber, R. M. Brown, and P. Michael, BNL

OBJECTIVE:

1. To determine the ratio of pollutant transport that occurs below the mixing height to the total transport.
2. To determine whether the pollutant mix is the same above and below the mixing height.
3. To document diurnal changes in the pollutant profile and on a time scale of changes in the synoptic situation.
4. To compare methods of defining the mixing height.

RESEARCH PLAN: Pollutant profiles will be obtained using a research aircraft in the early morning and late afternoon, within and outside of the pall from New York City. Approximately four experiments will be performed within a one-week period. Experiments will be done at various times of the year. Detailed profiles of particulates, SO_2, temperature, dew point, wind speed and direction will be measured. In addition, filter samples will be taken at four altitudes and analyzed for SO_2, sulfates and trace metals (via CPXE).

FIELD LOCATION: Vicinity BNL and New York City, N. Y.

FIELD EXPERIMENT TIMETABLE: December 1977; Spring 1978; Summer, 1978; Fall 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Two Years

TASK 4: Pollutant Distribution

SUB-TASK: 3. Size Discriminatory Chemical Analysis of Suboptical Particles

CONTACT: Roger L. Tanner and William H. Marlow, BNL

OBJECTIVE: Determination of size distributions (and variability thereof) of chemically speciated, airborne sulfate samples in a variety of geographical locations, seasons and meteorological conditions using low and high volume diffusion samplers and other variations of the technique.

RESEARCH PLAN: Application of the diffusion-sampling method will be made in a variety of locations and temporal formats with emphasis in three areas: (1) extended 12 hour, low volume experiments in several locations, seasons; (2) half-hour, high volume sampling from an airborne sampler combining virtual and slit-to-cylinder impactor stages with a diffusion sampler; (3) cyclical sampling of diffusion battery stages with a real-time flame-photometric analyzer for highly time-resolved airborne sulfate size distribution.

FIELD LOCATION: Aircraft, research ground stations

FIELD EXPERIMENT TIMETABLE: Mid-77 - continuing

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Tanner, R. L. and W. H. Marlow, "Size Discrimination and Chemical Composition of Ambient Airborne Sulfate Particles by Diffusion Sampling," *Atmos. Environ.*, 1977 (in press).

TASK 4: Pollutant Distribution

SUB-TASK: 4. Characterization Flights

CONTACT: R. W. Garber, R. M. Brown, BNL

OBJECTIVE: To form a base of information on the character of the atmosphere in predetermined volumes over fixed time periods in the Northeast United States.

RESEARCH PLAN: A series of regional scale characterization flights will be made during 1977-1978 to establish realistic information on the transport and transformation of material within specific areas in the Northeast United States. Some of the flights will take place during the SURE intensive measurement periods and will cover the region from Brookhaven, Long Island; Delmar, Maryland; Scranton, Pennsylvania and Montague, Massachusetts.

Two HORIzontal SCOPing Experiments (HORISCOPE) were made on March 30 and April 1, 1977 to determine the degree of temporal variability of atmospheric material and gases measured over horizontal traverses extending to regional scales (200 kilometers).

The HORISCOPE results were used as an aid to establish definite characterization flight plans including horizontal and vertical traversing, parameters to be measured, instruments to be used, filter sampling times, analytical procedures and computer analysis.

The first full scale characterization flights are scheduled for August 1977.

FIELD LOCATION: Northeastern United States

FIELD EXPERIMENT TIMETABLE: First flights will be in August 1977, then subsequently as needed to interface with extensive regional sampling periods.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: 2-3 years

TASK 4: Pollutant Distribution

SUB-TASK: 5. Quality Assurance of Analytical Results from the SURE Contractor.

CONTACT: Philip W. Krey, EML

OBJECTIVE: To evaluate the reliability of sampling and analyses of pollutants in surface air reported by the monitoring network of the Sulfur Regional Experiment (SURE).

RESEARCH PLAN: From each of about 20 sites of the SURE, EML will analyze each year half of 4 aerosol filters for energy-related pollutants of interest and compare results with the other half of the filter which will be analyzed by the Electric Power Research Institute (EPRI) contractor. EML will visit about 6 of the SURE sites and perform short-term (several days) aerosol and gas sampling for comparison with the contractor's results. Gases to be analyzed include SO_2, O_3, NO, NO_x and SF_6 if desirable.

FIELD LOCATION: To be decided.

FIELD EXPERIMENT TIMETABLE: Two SURE sites will be visited in FY-1977 and four sites in FY-1978.

REPORTING ORGANIZATION: Environmental Measurements Laboratory

PROJECT DURATION: FY-1977 and FY-1978

TASK 5: Pollutant Transport

SUB-TASK: 1. Planetary Boundary Layer Studies

CONTACT: B. B. Hicks and T. Yamada, ANL

OBJECTIVE: To obtain a continuous, long-period record of the characteristics of the planetary boundary layer, including documentation of such features as fine-scale temperature and wind profiles, and turbulence intensities.

RESEARCH PLAN: As a sequel to the 1975 and 1976 ANL "Sangamon" studies, to monitor the evolution of the PBL over about a four-day period using the high-resolution WHAT system coupled with free-rising radiosondes and captive balloon packages, together with at least one monostatic acoustic sounder. The experiment is planned to take place during October 1977, in conjunction with the cooperative "AMBIENS" experiment. Particular attention will be given to the process of decoupling of air aloft from the surface boundary layer.

FIELD LOCATION: Midway between Rushville and Shelbyville, Indiana, in Rush County.

FIELD EXPERIMENT TIMETABLE: October, 1977

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: One week experimental period plus extensive analysis.

TASK 5: Pollutant Transport

SUB-TASK: 2. AMBIENS Experiment

CONTACT: B. B. Hicks, ANL

OBJECTIVE: To test contemporary descriptions of the behavior of sulfur compounds in the lower atmosphere through an experimental investigation of the Atmospheric Mass Balance of Industrially Emitted and Natural Sulfur (AMBIENS).

RESEARCH PLAN: A cooperative study will take place in Southern Indiana during October 1977. Two or more aircraft will take part, flying legs of a 100 km box pattern in a highly polluted area void of significant sources. The experiment will take place during south-westerly flow, so that the large sulfur sources located along the Ohio River valley will be largely upwind, although at a sufficient distance that individual plumes will be difficult to detect. Supporting PBL observations at a site located within the box (at a location midway between Shelbyville and Rushville, Indiana) will concentrate on monitoring the structure of the planetary boundary layer by use of free-rising radiosondes and remote-sensing acoustic sounders.

FIELD LOCATION: Southern Indiana

FIELD EXPERIMENT TIMETABLE: October 1977

REPORTING ORGANIZATION: Argonne National Laboratory

COOPERATING ORGANIZATIONS: BNL, PNL, SRI, EMI, LLL

PROJECT DURATION: Two weeks

TASK 5: Pollutant Transport

SUB-TASK: 3. Development of Long-Range Tracer System

CONTACT: Gilbert J. Ferber, ARL

OBJECTIVE: To develop instrumentation and techniques for release, sampling, and analysis of perfluorocarbons and to determine the feasibility of their use in atmospheric dispersion experiments over distances from about 100 to 1000 km.

RESEARCH PLAN: Results of the first field test (April 1977) of the perfluorocarbon tracer system will be evaluated. Two perfluorocarbons (C_6F_{12} and C_8F_{16}) were released simultaneously with two heavy methanes and SF_6. Over 100 air samples, collected at 3, 50 and 90 km from the release point, will be analyzed and tracer ratios determined to test the reliability of procedures used for release, sampling and analysis, and to verify the conservative nature of the tracers in the atmosphere.

Performance of 3 different prototype perfluorocarbon samplers will be evaluated and any necessary modifications will be made. Recommendations will be made this summer concerning near-term use of perfluorocarbons in a field experiment and for longer-term development of tracer systems.

FIELD LOCATION: Site of future experiment is yet to be selected.

FIELD EXPERIMENT TIMETABLE: Target date for earliest use of perfluorocarbon tracers in a MAP3S experiment is Fall 1978.

REPORTING ORGANIZATION: NOAA-Air Resources Laboratory

COOPERATING ORGANIZATIONS: EML, BNL

PROJECT DURATION: Through FY-1978

REFERENCES: Report on recent tracer tests in preparation.

TASK 5: Pollutant Transport

SUB-TASK: 4. Measurement of Long-Range Tracer Compounds for New Atmospheric Tracer Systems

CONTACT: R. N. Dietz, BNL

OBJECTIVE: Verify performance of tracer compounds and employ sampling and analysis techniques in field material balance and long-range tracer experiments.

RESEARCH PLAN: SF_6 and other tracer release experiments are planned to evaluate release techniques, new automatic sampling bottle stations, and low flow (less than 1 cm^3/min) critical orifices. These experiments will be precursors to our participation in the MAP3S Box Budget Experiment this fall.

Special detector techniques will be employed to improve the limit of detection of the continuous monitor to levels of about 0.05 ppt.

Concentrating air samplers based on molecular sieve adsorbents will be developed for continuous, unattended sampling of multiple tracers. With a drying agent ahead of less than 0.1 g of 13 X molecular sieve, more than 10 liters of air could be passed through with no break-through of perfluorocarbons.

DEVELOPMENT STATUS: An aircraft mountable SF_6 sampler is available, perfluorocarbon sampling devices are progressing.

PLANNED AVAILABILITY: SF_6 sampler will be available in the summer 1977, perfluorocarbon sampler availability is expected in 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Dietz, R. N., E. A. Cote, and R. W. Goodrich, "Ultratrace Determination of Sulfur Hexafluoride and Perfluorocarbons for Atmospheric Tracing," Abstract, ACS Meeting, Chicago, IL, August 1977.

Dietz, R. N., E. A. Coté and R. W. Goodrich, "Air Mass Movements Determined by Real-Time Frontal Chromatography of Sulfur Hexafluoride," in *Measurement, Detection and Control of Environmental Pollutants*, IAEA-SM-206/21, September 1976, pp. 277-299.

TASK 6: Pollutant Transformation

SUB-TASK: 1. ^{18}O Enrichment of Atmospheric Sulfate, Sulfur Dioxide, and Water Vapor.

CONTACT: P. Cunningham and R. Kumar, ANL

OBJECTIVE: Simultaneously collect samples of atmospheric sulfate, sulfur dioxide, water vapor, and dust fall in a form suitable for oxygen isotope ratio analyses.

RESEARCH PLAN: Using a suitable sampling system, such as a filter for the atmospheric sulfate, an alkaline filter for the sulfur dioxide, a chilled surface for the water vapor, and a dry or wet dust collector, weekly samples will be collected at one or more sites in the MAP3S region. Possible correlations between the ^{18}O enrichments of the various species collected will be investigated; seasonal variations in the ^{18}O enrichments in the individual species will be determined.

FIELD LOCATION: To be arranged

FIELD EXPERIMENT TIMETABLE: To be determined

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: Two years

REFERENCES:

Cunningham, P. T. et al., "Chemical Engineering Division Environmental Chemistry Annual Report, July 1974-June 1975," ANL-75-51, 1975.

TASK 6: Pollutant Transformation

SUB-TASK: 2. Mechanics of Aerosol Particulate Interactions

CONTACT: W. H. Marlow, BNL

OBJECTIVE: Characterization of different general aspects of aerosol mechanics and interactions.

RESEARCH PLAN:

A. Investigate possibility that aerosol charging (cluster ion acquisition) may be a good physical model for aerosol capture of extremely fine particles (molecular clusters), thus enabling rate determination of capture for model calculations of aerosol coagulation.

B. Develop stochastic theory of aerosol charging following guidelines laid down recently.

DEVELOPMENT STATUS: Problem has been isolated and formulated. Specific aspects of solution yet to be investigated before calculations can be done.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Marlow, W. H., "Unipolar Aerosol Diffusion Charging, I: Introduction and Charging of High and Low Dielectric Constant Monodisperse Aerosols by Time-Invariant Ion Distributions," *J. Colloid Interface Sci.*, 1978 (in press).

Marlow, W. H., "Unipolar Aerosol Diffusion Charging, II: Ion and Aerosols Polydispersities in Unipolar Charging the 'Diffusion Charging Mobility Analysis' Hypothesis," *J. Colloid Interface Sci.*, 1978 (in press).

Marlow, W. H., "Calculations of Unipolar Aerosols Charging," in *Colloid and Interface Science, Vol. II: Aerosols, Emulsions and Surfactants*, Milton Kerker (ed.), Academic Press, 1976.

TASK 6: Pollutant Transformation

SUB-TASK: 3. Fundamental Studies of Aerosol Formation, Interaction, and Growth Processes.

CONTACT: W. Marlow (BNL) and J. R. Brock (U. of Texas)

OBJECTIVE: Develop the mathematical tools whereby specific aerosol processes can be understood and generalized.

1. Molecular dynamics and Monte Carlo calculations of aerosol processes.
2. Characterization of composition-dependent forces between particles and between particles and molecules.

RESEARCH PLAN:

1. Extension of earlier work to calculate coagulation rates between particles in transition regime.
2. Condensation calculation in the transition regime - Monte Carlo study of condensation for realistic masses for condensible gas species.
3. H_2O-H_2 SO_4 cluster description - assessment of feasibility for using numerical techniques of quantum chemistry.
4. Role of van der Waals forces in interparticle interactions.

DEVELOPMENT STATUS: In development

PLANNED AVAILABILITY: Several years

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Harrison, H., "A Molecular Dynamics Study of Dimer Formation," Ph.D. Dissertation, University of Texas, 1972.

TASK 6: Pollutant Transformation

SUB-TASK: 4. Airborne Plume Studies

CONTACT: L. Newman and R. W. Garber, BNL

OBJECTIVE: Further studies on the oxidation of SO_2 and the formation of $SO_4^=$ species in the emissions and plumes from energy related point sources, e.g. fossil fueled electric generating stations.

RESEARCH PLAN: Study the chemical transformations in plumes from fossil fueled power plants to gain an understanding of the oxidation of SO_2 and the resultant formation sulfate species. The study will be conducted by the BNL aircraft. Typical operations will consist of sampling the emissions in the plume at several downwind distances (e.g., 1, 3, 10, 30 miles) and measuring the sulfate to total sulfur ratio at the selected locations. The principal measurements will utilize the BNL filter pack to obtain integrated samples of sulfate aerosol and sulfur dioxide. Concurrent real-time measurement of gaseous pollutants and aerosols will be made. Experiments will be conducted during a reasonable variety of meteorological conditions including high and low temperature and humidity regimes as well as day and night. Heterogeneous and homogeneous reaction mechanics will be addressed.

FIELD LOCATION: Selected power plants in the northeastern United States.

FIELD EXPERIMENT TIMETABLE: Initial studies in the spring of 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: 3 years

REFERENCES:

Newman, L., J. Forrest and B. Manowitz, "The Application of Isotopic Ratio Technique to a Study of the Atmospheric Oxidation of Sulfur Dioxide in the Plume from an Oil-Fired Power Plant," *Atmos. Environ.*, *9*, 959, 1975.

Newman, L., J. Forrest, and B. Manowitz, "The Application of an Isotopic Ratio Technique to a Study of the Atmospheric Oxidation of Sulfur Dioxide in the Plume from a Coal-Fired Power Plant," *Atmos. Environ.*, *9*, 969, 1975.

Schwartz, S. E. and L. Newman, "Processing Limiting Oxidation of Sulfur Dioxide in Stack Plumes," *Environ. Sci. and Tech.*, 1977 (in press).

TASK 6: Pollutant Transformation

SUB-TASK: 5. Modeling Homogeneous and Heterogeneous SO_2 Oxidation

CONTACT: S. E. Schwartz and S. Z. Levine, BNL

OBJECTIVE: Develop models for SO_2 oxidation which will allow incorporation of salient features of homogeneous gas-phase and heterogeneous reactions into integrated chemical-meteorological simulation model.

RESEARCH PLAN: SO_2 may be oxidized in homogeneous gas-phase reactions by several free radicals, HO, HO_2, RO_2, and $RCOO_2$, whose concentrations depend on the concentrations of numerous other atmospheric constituents including NO, NO_2, O_3, H_2O and hydrocarbons, as well as upon insolation. At the present time homogeneous SO_2 chemistry appears to be adequately treated by a reaction scheme incorporating some 30 constituents; however, a substantial reduction in the number of modeled species will be necessary to meet the constraints of integrated chemical-meteorological models. This reduction will be achieved by a parameterization of the concentrations of the relevant chemical compounds in terms of several directly modeled species. In this effort we shall make use of experience gained with the larger reaction system to examine steady-state concentrations, concentration ratios, etc.

Modeling activity for heteorogeneous SO_2 oxidation consists at present of an examination of the rate of aqueous-phase reactions, pertinent to in-cloud or aerosol processes, as governed largely by temperature and the concentrations of trace metals, NH_3, and H_2O.

It is to be stressed that the chemical modeling activity derives heavily upon experimental research being conducted both within and outside the MAP3S community, and will be maintained as flexible as possible so that the results of this research may be incorporated. The modeling activity described herein will be conducted in close coordination with the meteorological modeling activities at Brookhaven and elsewhere within the MAP3S modeling community.

DEVELOPMENT STATUS:	A single box numerical model dealing with a relatively complete set of reactions is operational. A reduced set of reactions is being investigated including homogeneous processes.
PLANNED AVAILABILITY:	A reduced reaction set treating homogeneous processes should be available for use in models during 1978.
REPORTING ORGANIZATION:	Brookhaven National Laboratory
PROJECT DURATION:	2-3 years

TASK 6: Pollutant Transformation

SUB-TASK: 6. Plume Transformation Study

CONTACT: A. J. Alkezweeny and J. M. Hales, PNL

OBJECTIVE: Determination of parameters describing pollutant transformations in urban plumes (and imbedded power plant plumes) for subsequent use in regional modeling efforts.

RESEARCH PLAN: This project is totally dedicated to the MAP3S program. As such it attempts to take a responsive stance toward joint, inter-laboratory projects while maintaining a high level of performance within earlier experiment designs, which are primarily of a single-laboratory nature. Within this capacity, this project expects to participate in the following studies during the coming year:

1. Further box-budget studies of the AMBIENS type, on a multi-laboratory cooperative basis;
2. Continued Lake Michigan plume transformation flights, under the design of the ongoing Long Range Plume Transformation Study;
3. Possible further flights over Lake Erie, in cooperation with Environment Canada.

FIELD LOCATION: Muskegon, Michigan and elsewhere in the MAP3S region.

FIELD EXPERIMENT TIMETABLE: Open: Multi-laboratory studies
Summer 1978: Long-range plume flights.

REPORTING ORGANIZATION: Battelle-Pacific Northwest Laboratory

PROJECT DURATION: Continuing

TASK 7: Surface Removal Processes

SUB-TASK: 1. Dry Deposition Studies

CONTACT: B. B. Hicks and M. L. Wesely, ANL

OBJECTIVE: Parameterization of the atmospheric and surface properties that affect gaseous and particulate deposition rates at the surface of the earth.

RESEARCH PLAN: The plan is to take numerous measurements over various surfaces to determine deposition rates for gases and particles. Standard micrometeorological supporting measurements will be taken in all cases. Measurements of the important surface properties will be made, including physiological characteristics of the plants if necessary. Initial emphasis will be placed on study of the properties of soybeans that affect sulfur dioxide uptake. Cooperative measurements by ecologists should help establish dose-response relationships of soybeans. Since ozone effects are expected to interfere, ozone fluxes will also be estimated. During the summer of 1977, a short-term study of fluxes above a forest will be performed also. This study funded cooperatively by EPA.

FIELD LOCATIONS: Illinois rural sites, Duke Forest, North Carolina

FIELD EXPERIMENT TIMETABLE: Summer 1977: field study over soybeans
Summer 1977: field study over forest
Winter 1977-78: field study over winter grass
Summer 1978: field study over soybeans and corn
Winter 1978-79: field study over winter surfaces
Summer 1979: further field studies

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: 2-4 years

TASK 8: Wet Removal Processes

SUB-TASK: 1. MAP3S Precipitation Chemistry Network

CONTACT: T. Dana, J. E. Rothert, D. W. Glover, and D. R. Drewes, PNL

OBJECTIVE: Operation of a network of wet-deposition-only precipitation collectors in the MAP3S region. Precipitation event samples are analyzed and the results reported monthly and semiannually.

RESEARCH PLAN: Four sites have been operating since December 1976 (at the latest), collecting event samples which are delivered promptly to and analyzed by Battelle-Northwest. Monthly reports of concentration data have been issued since January 1977, and the first periodic summary report will be issued in late 1977.

The field data collected and reported include: duration of sample, duration of precipitation event, time and date of collection, sample volume, predicted sample volume, number of collector openings, and field sample pH. Laboratory data include pH and conductivity, and concentrations of: SO_2 (dissolved), $SO_4^{=}$, NH_4^{+}, NO_2^{-}, NO_3^{-}, Cl^{-}, PO_4^{3-}, Na^{+}, K^{+}, Mg^{++}, Al^{3+}, and Ca^{++} All the ions are analyzed by ion chromotography, except Mg, Al, and Ca, which are done by atomic absorption spectrophotometry, and SO_2 and NO_2^{-}, which are done by Technicon Autoanalyzer methods.

In accordance with the primary objectives of the project, sampling of precipitation events, rapid chemical analyses, and monthly reporting of concentration data will continue. With the deployment of three new sites (to a current total of seven), however, event sampling will normally be conducted only with the Battelle collector, and the sampler comparison study will be conducted at one site only (Penn State). This study will involve event sampling with nine collectors: three each of Battelle, EML-type, and the Sangamo-type as used on the Canada Atmospheric Environment Service Network. The comparison study should begin during the early 1978 and proceed until a statistically significant number of event samples is collected; the emphasis in comparison will be on the sulfur species $SO_3^{=}$ and $SO_4^{=}$, but the regular list of species will be analyzed.

EML or EML-type collectors in service at the other sites will be shifted to a weekly sampling schedule when the one-site study begins. This schedule will match that of the Department of Agriculture network, some of which may coincide with the current MAP3S sites.

FIELD LOCATIONS: State University of New York at Albany, Cornell University, Pennsylvania State University, University of Virginia, ISWS, BNL, University of Delaware.

FIELD EXPERIMENT TIMETABLE: The network will expand from 4 to 8 sites in late 1977.

REPORTING ORGANIZATION: Battelle-Pacific Northwest Laboratory

PROGRAM DURATION: Continuing

REFERENCES:

Dana, M. T., D. R. Drewes, D. W. Glover, J. M. Hales and J. E. Rothert, "The MAP3S Precipitation Chemistry Network," in *Pacific Northwest Laboratory Annual Report for 1976 to the ERDA Assistant Administrator for Environment and Safety, Part 3: Atmospheric Sciences*, pp. 101, BNWL-2100, Pt. 3, October 1977.

TASK 8: Wet Removal Processes

SUB-TASK: 2. Precipitation Sampling

CONTACT: G. S. Raynor, BNL

OBJECTIVE: Document constituents and characteristics of precipitation on Long Island and relate these to pertinent meteorological factors and pollutant source distribution. Also investigate drop size distribution during each rainfall.

RESEARCH PLAN: Sample all precipitation events each hour using automatic, sequential precipitation collector. Analyze samples for chemical constituents. Relate data to meteorological factors and pollutant source distribution. Separate rainout from washout. Measure drop size distribution with Illinois State Water Survey instrument.

FIELD LOCATION: Brookhaven National Laboratory

FIELD EXPERIMENT TIMETABLE: In progress. To continue indefinitely.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: Continuing

REFERENCES:

Raynor, G. S., "Meteorological and Chemical Relationships from Sequential Precipitation Samples," BNL Report No. 22879, 1977.

TASK 8: Wet Removal Processes

SUB-TASK: 3. East-Central Illinois Precipitation Sampling Station

CONTACT: G. J. Stensland

OBJECTIVE: To examine the causative factors of variable precipitation chemistry, including pH, in a rural region, and initiate a continuous, long-term sampling station.

RESEARCH PLAN: A precipitation sampling station has been installed near Champaign, Illinois, incorporating a variety of samplers and meteorological equipment. One of the MAP3S rain samplers is scheduled to be installed at the site in late summer or early fall. This station is of particular interest since sporadic data are available since the middle 1950's allowing a trend to be studied. It is likely that the site will also be included in the USDA network to be implemented in early fall. The time scale of sampling will extend from less than a minute per sample (sequential) to weekly allowing comparisons between various sampling modes. The wide variety of samplers available will be used to evaluate various instruments.

FIELD LOCATION: Vicinity of Champaign-Urbana, Illinois

FIELD EXPERIMENT TIMETABLE: Sampling will start in the fall of 1977.

REPORTING ORGANIZATION: Illinois State Water Survey

PROJECT DURATION: Long term

TASK 8: Wet Removal Processes

SUB-TASK: 4. Chicago Area Field Project

CONTACT: R. G. Semonin, ISWS

OBJECTIVE: To collect air and precipitation samples for chemical analysis of AER and non-AER constituents in a large region surrounding the south Lake Michigan basin. To ascertain the spatial variability of AER and non-AER pollutants on a sub-MAP3S grid scale.

RESEARCH PLAN: Installation and operation of a grid of rain-only samplers interspersed with wet/dry collectors, sequential collectors, air samplers, and drop size spectrometers. The samples will typically consist of weekly exposures during all seasons of the year with intermittent short duration intensive collection periods. The stations will be so located as to indicate the contribution of the Chicago area industrial centers to the air and precipitation quality in the region out to > 200 km.

FIELD LOCATION: Region surrounding south Lake Michigan basin.

FIELD EXPERIMENT TIMETABLE: Cooperation of the State of Illinois, NSF, Governor's State University, Northern Illinois University, Purdue University, Western Michigan University and Michigan State University has been obtained. The network will be set-up during 1978.

REPORTING ORGANIZATION: Illinois State Water Survey

PROJECT DURATION: 3 years from start date

TASK 8: Wet Removal Processes

SUB-TASK: 5. Source Identification of AER Pollutants

CONTACT: D. F. Gatz, ISWS

OBJECTIVE: To identify, through factor analysis, the relationship between analyzed species and suspected sources.

RESEARCH PLAN: Factor analysis allows interpretation of air and rain chemistry data with regard to source terms. Meteorological variables, specifically wind, and the correlation between specific trace metals are used to estimate the source type (metal processing, fuel burning, autos, etc.). This analysis when coupled with emission data is useful to discern the contribution at a receptor from a source of a specific element or compound.

FIELD LOCATION: Region surrounding the south Lake Michigan basin

FIELD EXPERIMENT TIMETABLE: Data from the area surrounding Chicago should be available for analysis beginning in late 1978.

REPORTING ORGANIZATION: Illinois State Water Survey

PROJECT DURATION: 3 years from start date

TASK 8: Wet Removal Processes

SUB-TASK: 6. Agricultural Impacts of Wet/Dry Deposition

CONTACT: R. G. Semonin, ISWS

OBJECTIVE: Utilizing agronomy and agro-economic skills to assess the presumed impact of air and rain quality on crop yields, and regional production.

RESEARCH PLAN: Using field measurements of AER pollutants in air and rain, in-the-field inspection of crops in suspected impact areas will be compared with control fields. The initial effort will focus on those crops (yet to be determined) most susceptible to yield alteration.

FIELD LOCATION: Region surrounding south Lake Michigan basin.

FIELD EXPERIMENT TIMETABLE: In cooperation with the State of Illinois, University of Illinois, and Purdue University, studies will begin as soon as data start to become available in 1978.

REPORTING ORGANIZATION: Illinois State Water Survey

PROJECT DURATION: 3 years from start date

TASK 8: Wet Removal Processes

SUB-TASK: 7. Precipitation Scavenging

CONTACT: B. C. Scott and J. M. Hales, PNL

OBJECTIVE: Determination of wet-removal parameters necessary for formulation of reliable regional models of pollution behavior.

RESEARCH PLAN: The plan for obtaining the objectives stated above is composed of two major steps, which are outlined as follows:

Step 1: Utilization of relatively simple lake effect storms as experiment systems to evaluate some of the unknown microphysical phenomena important for determining scavenging parameters. The Lake Michigan area will be utilized for these experiments; resulting data will be analyzed with the use of comprehensive numerical models of storm-dynamics behavior.

The lake-effect storm scavenging experiment, as indicated in Fig. 3, is designed about a macroscopic material-balance framework. Thus, the PNL aircraft will inventory pollution inflow and release tracers in the upwind region, and subsequently monitor outflow downwind. A ground based precipitation sampling network will provide a measure of precipitation removal. Although this is at a preliminary planning stage, it is hoped that the joint experiments of the University of Chicago and Illinois State Water Survey will provide additional cloud physics, precipitation chemistry, and radar information for the project.

Step 2: Utilizing the information generated in Step 1 to evaluate behavior in general cyclonic storm systems. Field studies will be conducted in such systems and will be interpreted with the aid of mesoscale moist modeling efforts. Parameters derived from these analyses will be of direct use for inclusion in regional prognostic models.

FIELD LOCATION:	Muskegon, Michigan
FIELD EXPERIMENT TIMETABLE:	Winter 1976: Preliminary measurements, lake storms
	Winter 1977: Comprehensive lake storm experiments
	1978-79: Lake and cyclonic storm experiments
REPORTING ORGANIZATION:	Battelle-Pacific Northwest Laboratory
PROJECT DURATION:	Continuing

LAKE MICHIGAN
POLLUTION INFLOW
BATTELLE DC-3
INFLOW POLLUTANT MONITORING
AND TRACER RELEASE
DOPPLER RADAR
AIR TRAFFIC RADAR
FAA MUSKEGON
WEATHER RADAR (PPI, RHI)
NWS
GROUND SITES
SEQUENTIAL IMPACTORS
AND PRECIP COLLECTORS
DOPPLER RADAR
U OF CHICAGO AIRCRAFT
CLOUD PHYSICS
PRECIPITATION SAMPLING
NETWORK
U OF MICH., BNW
BATTELLE DC-3
OUTFLOW POLLUTANT
MONITORING
CAP PRECIPITATION
SAMPLING NETWORK
(PROPOSED)
ISWS

FIGURE 3.

TASK 9: Weather and Climate Modification

SUB-TASK: 1. Turbidity Experimental Network

CONTACT: M. L. Wesely, ANL

OBJECTIVE: To determine the extent of regional-scale episodes of increased haze in the northeastern United States and to assess the associated changes in solar radiation.

RESEARCH PLAN: During the summer of 1977, a preliminary analysis of the data sent from the ten sites in the Northeast at which atmospheric turbidity is being measured will be performed. The temporal and spatial patterns of haze will be studied, and compared to turbidity variations measured in the past. In consideration of the expanded DOE/NOAA solar radiation network, some of the site locations may be altered after the summer of 1977 to most effectively use resources available. Ultimately, the changes in diffuse and direct solar radiation components due to haze will be estimated for the Northeast, and the effects of the corresponding changes in effective albedo will be examined.

FIELD LOCATION: BNL; Burlington, VT; Oxford, OH; ORNL; St. Louis; Manhattan, KS; Guelph, Ontario (in cooperation with the Atmospheric Environment Service of Canada); Pellston, MI; University Park, PA; Charlottesville, VA.

FIELD EXPERIMENT TIMETABLE: Data collection and preliminary analysis during 1977 and 1978. Reevaluation of site locations in late 1977, with changes of site locations, if necessary.

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: 2 years

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 1. Model Development

CONTACT: D. C. Powell and L. L. Wendell, PNL

OBJECTIVE: To determine the feasibility of making the Lagrangian model more realistic by treating the aspects of diffusion, transformation and wet and dry removal each with more sophisticated techniques.

RESEARCH PLAN: The plan for accomplishing the objective, stated above, is to be carried out in separate steps which are briefly listed below.

Step 1: Incorporate the capability into the model to accept hourly gridded values of mixing depth and stability class which have been generated with sounding and hourly surface data.

Step 2: Incorporate more complex chemistry within the plume involving more than two species as well as the capability of chemical reaction between the plume and its environment.

Step 3: Incorporate the precipitation chemistry into the model for validation with the precipitation chemistry network.

Step 4: Incorporate into the model the capability to keep track of short-term (down to hourly) maximum air concentrations as well as precipitation chemistry (acidity) in each grid square of the sampling grid. This capability will be used to compare concentrations from distant sources to those generated with a mesoscale model within an 80 km radius of a single source.

Step 5: Test the representativeness of calculating the precipitation scavenging using bulk parameters instead of representative dropsize distribution and particle size distributions.

Step 6: Evaluate the space and time resolution requirements of the real-time precipitation data.

Step 7: Conduct sensitivity tests with the model for varying degrees of sophistication and different lengths of assessment time.

DEVELOPMENT STATUS:	The existing model is being improved to meet the requirements stated in the Research Plan.
PLANNED AVAILABILITY:	Features for model improvement will be made available to other laboratories as they are tested and determined to be essential for improved assessments.
REPORTING ORGANIZATION:	Battelle-Pacific Northwest Laboratories
PROJECT DURATION:	18 months

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 2. Case Study Verification with Comprehensive Data Sets

CONTACT: L. L. Wendell, D. J. McNaughton, and D. C. Powell

OBJECTIVE: To establish two or three benchmark cases of the most comprehensive meteorological and air quality data available and to conduct verification exercises to investigate model reliability.

RESEARCH PLAN: The plan for accomplishing the stated objectives contains two steps which are described below:

Step 1: Obtain meteorological data consisting of the two or three NASA data sets of 3-hourly radiosonde data, the corresponding surface data, and hourly precipitation data along with output data sets from Carl Kreitzberg's three-dimensional dynamic model. The air quality data collected for this sub-task would consist of power plant emission data from the Federal Power Commission, emission inventories from the EPA, air quality measurements from the EPA, as well as air quality measurements from EPRI and state agencies. These data sets would be compiled in close cooperation with the BNL Data Management Program and would reside in their file for use in any model verification exercise.

Step 2: Once the data sets were suitably formatted and compiled they would be used to test the sensitivity of the transport schemes of the PNL single layer and eight layer models to the time resolution of the radiosonde data. The data from Kreitzberg's model would be used for comparison with the vertical as well as horizontal transport produced in the eight layer isentropic-diabatic model. The pollution source and air quality data would be carefully examined to select the most effective way to conduct a verification exercise of the model's transformation and removal processes.

DEVELOPMENT STATUS: Data are being gathered.

PLANNED AVAILABILITY:	Data set in 6 months, models 18 months.
REPORTING ORGANIZATION:	Battelle-Pacific Northwest Laboratory
PROJECT DURATION:	1-2 years

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 3. Gaussian Puff Model with Wind Shear

CONTACT: C. M. Sheih

OBJECTIVE: To develop a regional-scale Gaussian puff model with consideration of wind shear.

RESEARCH PLAN: Available puff or plume models for regional areas neglect wind shear. However, it is generally agreed that wind shear could be an important factor in dispersing pollutants over regional scales because of the size to which pollutant clouds will grow. Schemes that include a description of the vertical wind shear have been developed by many investigators, and methods for including horizontal variations have recently been developed at ANL. The present plan is to incorporate these schemes in a Gaussian puff model for simulating sulfur pollution over the region of interest to MAP3S.

DEVELOPMENT STATUS: In progress

PLANNED AVAILABILITY: 1978

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: One year

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 4. Trajectory Modeling of Long-Range Transport

CONTACT: J. L. Heffter, ARL

OBJECTIVE: Verification of accuracy of numerical simulations of long range transport (to $\sim$ 1000 km) of pollutants.

RESEARCH PLAN: Two years of hourly meteorological data from all reporting surface stations within the boundaries 20-50°N latitude and 60-100°W longitude is now available at NCC-Asheville, N. C.

These data are being incorporated into both the regional-continental scale and mesoscale models.

Model verification will be performed using observed surface air concentrations such as those taken in the Savannah River Kr-85 weekly and twice daily measurement programs.

DEVELOPMENT STATUS: Undergoing continued verification

PLANNED AVAILABILITY: An operational version available now

REPORTING ORGANIZATION: NOAA-Air Resources Laboratory

PROJECT DURATION: On-going

REFERENCES:

Heffter, J. L. and G. J. Ferber, "The ARL Transport, Dispersion and Deposition Model and Model Verification Experiments," in *Preprints Volume, Joint Conference on Applications of Air Pollution Meteorology*, Salt Lake City, Utah, American Meteorological Society, Boston, MASS, 1977.

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 5. Finite-Difference Diffusion Model

CONTACT: C. M. Sheih, J. D. Shannon, and T. Yamada

OBJECTIVE: To develop a finite-difference model capable of simulating transport and transformation of pollutants over regional scales.

RESEARCH PLAN: The task is to develop a computer program which will describe the regional-scale characteristics of atmospheric pollution in the greater northeastern United States. The program will consist of a number of subroutines describing: (1) atmospheric dispersion and diffusion, (2) source terms, (3) meteorological fields, (4) deposition velocity maps, (5) chemical reactions, (6) precipitation scavenging, (7) topography, (8) high-order turbulent closure, and (9) graphic display requirements. These subprograms will be developed independently by several MAP3S participants. A high level of communications will be maintained in order to facilitate the exchange of new findings and the unification of the format of computer programming. The effort of ANL will focus primarily on items (1), (3), (4), (6) and (8).

DEVELOPMENT STATUS: Model development is underway based on the time schedule in the figure shown.

Computer Subprograms	Project Duration 1977	1978	1979	Investigators
Main Program				CMS
Numerical Scheme				CMS
Meteorological Scheme				CMS JDS & TY
Deposition Velocity Map				CMS
Precipitation Scavenging				TY
Higher-order Closure				TY
Topography				JDS

PLANNED AVAILABILITY: Model is expected to be available in 1979.

REPORTING ORGANIZATION: Argonne National Laboratory

PROJECT DURATION: 3 years

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 6. Regional Three-Dimensional Eulerian Diffusion-Advection Model with Nonlinear Chemical Reactions

CONTACT: R. E. Meyers, R. T. Cederwall, J. Storch, BNL

OBJECTIVE:

A. To develop a three-dimensional regional Eulerian grid transport, diffusion and chemical reaction (air quality) model for MAP3S.

B. To develop methods for examining and to evaluate the importance of including turbulence mixing in air quality models.

C. To establish a meteorological computer data link between National Weather Service, Suitland, MD and Brookhaven National Laboratory to be able to make near real-time air quality/meteorological calculations.

D. To develop an objective diagnostic method for improved analysis of meteorological fields needed for air quality calculations.

RESEARCH PLAN:

A. The following steps will be taken to develop the regional Eulerian air quality model:

1. Survey and critical analysis of existing methodologies;
2. Selection of candidate numerical methods and testing with respect to relative accuracies and acceptability;
3. Development of a model (with at least 3-hour time resolution, 32 km horizontal spatial resolution and variable vertical resolution) for MAP3S region;
4. Application of the above methodology to ERDA assessment problems.

B. Plume models will be developed using probability density concepts to incorporate chemical mixing properties of atmosphere. Model results will be compared against MAP3S and other plume measurements.

C. A DEC PDP 11/70 minicomputer at BNL will be linked to a dedicated transmission line between NWS, Suitland, MD and to the CDC computer system at BNL. Computer will acquire data from NWS, edit and archive

data and send data to CDC machines for model calculations. Equipment will be purchased, hardware will be assembled, and software will be developed or purchased.

D. A diagnostic method for improved analysis of meteorological fields will be developed using objective analysis methods and variational analysis using the equations of conservation of mass, momentum and total energy and employing the concepts of material layers and frontal analysis.

DEVELOPMENT STATUS:	Research in each area of the project plan has been initiated.
PLANNED AVAILABILITY:	The Suitland computer link should be available in mid-1978. Model development will continue into 1979.
REPORTING ORGANIZATION:	Brookhaven National Laboratory
PROJECT DURATION:	3 years

TASK 10: Numerical Modeling and Analysis

SUB-TASK: 7. Acquisition, Archiving, and Dissemination of Experimental Data Generated by MAP3S and Related Programs

CONTACT: C. Benkovitz, BNL

OBJECTIVE: To develop and implement a data bank for the MAP3S program that can serve as a central exchange facility for data collected by and needed by MAP3S researchers. A record of all MAP3S experiments and the data available from them will be kept in a MAP3S Experiment Index.

RESEARCH PLAN: The development of the computerized MAP3S Experiment Index will continue. User access will be both interactive and via requested reports. Further work will be done on the Experiment Report Forms and all MAP3S participants will be encouraged to send in their completed forms as soon as possible. Experience gained in this project will serve as a basis for the development of methodologies to handle experimental data not generated directly by MAP3S participants.

Cooperation with DOE's IWGDE and LWR Environmental Effects programs will continue so as to provide MAP3S participants in-house capability of creating and accessing ANSI standard format magnetic tapes.

Further work on data exchange with the EPRI SURE project will be pursued.

The development of summaries, graphs, maps, charts, etc. of experimental data being archived will be undertaken as soon as the initial problems of data flow and archiving are implemented and useful formats are defined.

DEVELOPMENT STATUS: The data bank structure has been developed and initial sets of data are being entered.

PLANNED AVAILABILITY: Data should start to be available from the MAP3S Data Bank in early 1978.

REPORTING ORGANIZATION: Brookhaven National Laboratory

PROJECT DURATION: 3 years

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APPENDIX: AGENCY AND PROGRAM ABBREVIATIONS*

AER - Atmospheric-Energy Related (pollutants)

AESC - Atmospheric Environment Service of Canada (Dr. Hans Martin)

ANL - Argonne National Laboratory (Mr. B. Hicks, Dr. P. Cunningham)

ARL - NOAA-Air Resources Laboratory (Dr. G. Ferber)

BNL - Brookhaven National Laboratory (Dr. P. Michael)

BYU - Brigham Young University (Dr. D. Eatough)

DBER - DOE Division of Biomedical and Environmental Research (Dr. D. Ballantine)

DOE - Department of Energy

EMI - Environmental Measurements, Inc. (Dr. L. Langan)

EML - Environmental Measurements Laboratory (Dr. P. Krey)

EPA - Environmental Protection Agency (Dr. P. Altshuller)

EPRI - Electric Power Research Institute (Dr. R. Perhac)

ERDA - Energy Research and Development Administration

ERT - Environmental Research and Technology, Inc.

FPC - Federal Power Commission

ISWS - Illinois State Water Survey (Dr. R. Semonin)

LBL - Lawrence Berkeley Laboratory (Dr. T. Novakov)

LILCO - Long Island Lighting Company

LLL - Lawrence Livermore Laboratory (Dr. M. MacCracken)

MAP3S - Multistate Atmospheric Power Production Pollution Study (Dr. M. MacCracken)

METROMEX - Metropolitan Meteorological Experiment (Dr. R. Semonin, ISWS)

MISTT - Midwest Interstate Sulfur Transport and Transformation Program (Dr. W. Wilson, EPA)

NEDS - National Emission Data System (EPA)

NOAA - National Oceanic and Atmospheric Administration

NSF - National Science Foundation

PNL - Battelle-Pacific Northwest Laboratory (Dr. J. Hales)

SRI - SRI, International (Dr. E. Uthe)

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*Where possible, a principal contact is given.

SUNY - State University of New York

SURE - Sulfur Regional Experiment (Dr. G. Hidy, ERT)

TDL - NOAA Techniques Development Laboratory

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