NOAA ARL Monthly Activity Report

July 2004

Bruce B. Hicks, Director
Air Resources Laboratory

Contents

Highlights

1. Highlight – Local Data Now Used in Plume Dispersion Forecasts. Data collected by the tower arrays set up by ARL in support of urban atmospheric research (DCNet, UrbaNet) can now be used in plume dispersion forecasting. The methodologies involved are not yet fully developed, but it is already clear that significant improvements in dispersion forecasts can be expected as the methodologies improve. The areas currently addressed are Washington, DC, and New York City. At this time, discussions are taking place to expand the number of urban areas being addressed, with the potential addition of Las Vegas and Fayetteville, North Carolina. Las Vegas is of interest because of its rapidly

growing air quality problem as well as its concerns about terrorism. Clark County, NV, in which Las Vegas resides, has requested attention to the issue from the NOAA Cooperative Institute for Atmospheric Sciences and Terrestrial Applications (CIASTA), with which ARL works closely. It is the terrorism concern that is driving thinking related to Fayetteville, where Fort Bragg is located. (Hicks, Pendergrass, Draxler)

2. Highlight – Evaluation of the Eta-CMAQ Air Quality Forecast Model: July 2004. An important component of this Air Quality Forecasting Program is the development and implementation of an evaluation protocol. Accordingly, a suite of statistical metrics that facilitates evaluation of both *discrete* forecasts (observed versus modeled concentrations of O_3) and *categorical* forecasts (observed versus modeled exceedances of the maximum 8-hr standards for O_3) are being calculated to characterize the performance of this model system. O_3 data from more than 600 monitors obtained from EPA's AIRNOW monitoring network are being used in the evaluation.

July results indicate that the system continues to perform fairly well, despite a continuation of the anomalously wet and cool conditions (unfavorable for the formation of ozone) that have dominated the region resulting in an average 8-hr maximum observed concentration of only 47.0 ppb (for the entire month). The model average of 57.3 ppb results in a Mean Bias (MB) of 9.9 ppb (Normalized Mean Bias = 21.8%). The average RMSE for the month was 16.0 ppb (Normalized Mean Error = 27.9%). Daily correlations for the month typically ranged between 0.40 and 0.70 (mean: 0.47), with better correlations occurring on the rare days when high pressure dominated the area. Because conditions were so unfavorable for O_3 formation, the number of exceedances that occurred during the month is very low. As a result, categorical statistics are not meaningful. (Brian Eder, 919.541.3994)

Silver Spring

3. HYSPLIT PC Training. The popularity of the HYSPLIT model has generated a demand for training. A comprehensive HYSPLIT training document has been created focusing on the PC version of the model. The 42 pages (one page per topic) include model configuration procedures, example graphical outputs, and discussion of the results. The training document is designed as a reference to be used in conjunction with an interactive demonstration of the modeling system. It provides additional examples to the ones shown in the on-line User's Guide. All aspects of the model are covered, from converting GRIB data to configuring the model for source attribution simulations. roland.draxler@noaa.gov

4. NOAA Workshops to Develop Options for Upper Air Observations for Climate. Plans are underway for a series of workshops to identify scientifically based and technologically attainable options for upper air observations to meet climate requirements that have been widely vetted within the climate community and other interested communities. Subject to change based on input from relevant internal NOAA committees, current plan calls for a series of three workshops focusing on (1) defining climate requirements for upper air observations, based on the full range of climate science needs, (2) assessing possible instruments and deployments to meet the requirements, and (3) developing options for upper air observations for climate in the context of other observing systems and national and international programs. A seven member organizing committee is planning the workshops, convened by the Chairs of the NOAA Research and Observing Systems Councils. dian.seidel@noaa.gov

5. Vertical Temperature Trends Assessment. Preparation of an assessment report on Vertical Temperature Trends in the atmosphere has begun, under the auspices of the US Climate Change Science Program. The report will address the discrepancies in temperature trend estimates between the surface and upper air and among different datasets. Dian Seidel is a lead author for chapter 2 of the report and is contributing datasets and computations for chapter 3. dian.seidel@noaa.gov

6. Global Radiosonde Temperatures Updated Through Spring. Global temperatures estimated from 63 and 54-station radiosonde networks have been updated through MAM of 2004. In general, there is little of moment to report, global surface and troposphere temperatures in this season about 0.5K above the 1961-1990 average and low-stratospheric temperatures remaining about 1.5K below this average. Only in the 300-100 mb tropopause layer is there obvious movement, the temperatures last spring in this layer rising above the 1961-1990 average for the first time since the El Chichon eruption in 1982. This tropopause-layer warming, beginning about 1995, is apparent in all seasons except summer, and represents one of the more interesting features of the atmosphere at the present time. (Jim Angell, 301 713 0295, x127)

Boulder

7. Refined Aerosol Optical Depth from SURFRAD/ISIS. Several advances have been made toward an aerosol optical depth (AOD) product for SURFRAD. The algorithm that uses the clear-sky identification data to calibrate the MFRSRs has been expanded from one channel (500nm) to all channels. The aerosol optical depth analysis program that applies those calibrations was also expanded to compute aerosol optical depth for all channels of the Multi-Filter Rotating Shadowband Radiometer. Dynamic station pressure acquisition from the SURFRAD data stream was also incorporated to compute molecular scattering for each two-minute AOD measurement. Similarly, a program to automatically access satellite-based total ozone from a Goddard Space Flight Center web site for the station and day being processed has been incorporated. This serves to more accurately compute the degree of ozone absorption for all channels. These latter two accomplishments are unprecedented in AOD analysis. Typically a mean station pressure is used for molecular scattering calculations. Last, a cloud-screening algorithm (also an SRRB product) was adapted to the new SURFRAD AOD calculations. Cloud screening of the daily AOD time series was the final hurdle to a SURFRAD AOD product. john.a.augustine@noaa.gov

8. Baseline Surface Radiation Network Meeting, Exeter, UK. Gary Hodges and Joe Michalsky attended the Baseline Surface Radiation Network biennial meeting in Exeter, UK, held this year at the UK Met Office. Gary presented posters "Grounding a BSRN station for protection from lightning-induced surges" and "SURFRAD: Surface radiation budget measurements for climate research and model and satellite validation." Joe gave an oral presentation entitled "Toward the development of a diffuse horizontal short-wave irradiance working standard." The SURFRAD program was mentioned early and throughout the meeting as a model for a well-run network providing useful data for model and satellite validation. The CUCF was also noted for its program to calibrate UV instrumentation and the fact that it has not yet been elevated to the World UV calibration facility. joseph.michalsky@noaa.gov

Oak Ridge

9. East Tennessee Ozone Study (ETOS). The ETOS intensive study began with six regional measurement sites on July 18, 2004. The pollutants measured are S02, HNO3, NO3, SO4 and O3. Ambient particulate (PM-2.5) monitors were deployed at two of these sites. A planned upgrade to twelve measurement sites will be conducted on August 1, 2004, with data collection beginning on August 2. Two additional ambient particulate monitors will be deployed on August 2. will.pendergrass@noaa.gov

Research Triangle Park

10. Community Multiscale Air Quality (CMAQ) Model - Ozone and Particulate Matter. Extensions to the 2003 public release version of the Community Multiscale Air Quality (CMAQ allows the tracking of primary elemental carbon and primary organic aerosol emitted from 16 source categories. This extended model has been coupled with Version 3 of the National Emissions Inventory (NEI) and run for a 10-day test period in June 1999. The results were compared with earlier model results based on Version 1 of the NEI, on a source-by-source basis. Estimates of particulate matter emissions from motor vehicles declined by 25% between Version 1 and Version 3 due to changes in the mobile-source activity and emission estimation methodologies. Estimates of biomass combustion emissions increased dramatically over the Southwest and Southeast due to improvements in spatial and temporal allocation of wildfires, prescribed forest fires, and agricultural burning. Carbon from coal combustion increased by a factor of 20 due to a speciation profile update. Predictions of emissions from the combustion of natural gas also increased significantly. The net effect of switching from Version 1 to Version 3 of NEI is a doubling of predicted summertime primary organic aerosol concentrations across most of the continental United States. This increase is also reflected in results of the 2001 year-long CMAQ model simulation. (Prakash Bhave, 919 541 2194; George Pouliot, 919 541 5475)

Developmental air quality forecasting of particulate matter distributions over the eastern United States was initiated on July 16, 2004. The Eta-CMAQ system is now being exercised in three streams: (1) experimental production of ozone forecasts over the northeast United States, (2) developmental forecasts of ozone over an expanded eastern United States domain, and (3) developmental forecasts of both O_3 and particulate matter over the expanded eastern United States domain. These provide opportunities to compare and contrast results from the different forecasts. Comparisons of the ozone forecasts over the northeast and eastern United States domains so far have indicated the influence of lateral boundary conditions in regulating the "modeled background" ozone levels and the need for accurate specification of lateral boundary conditions; accurate simulation of the "background" levels influences model performance during low-moderate ozone conditions. CMAQ-Eta forecasts of surface ozone from the northeast United States simulation are also being compared against measurements from the AIRMAP (Atmospheric Investigation, Regional Modeling, Analysis and Prediction) sites as well as with forecasts results from several other models as part of a model intercomparison conducted by the NOAA Aeronomy Laboratory for the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) field study.

Diagnostic simulations to assess the influence of top-down cloud mixing on predicted ozone distributions were continued. Previous analyses had indicated the role of ozone boundary conditions derived from the Global Forecast System (GFS) model and the subsequent downward mixing by deep

clouds on surface ozone levels. Sensitivity simulations involving limiting the diagnosed cloud tops to below the tropopause and those involving turning off downward mixing indicate the need for additional studies on: (1) maintaining consistency in various fields between the GFS, Eta, and CMAQ models (e.g., tropopause and associated dynamics), and (2) improving the representation of cloud mixing of atmospheric tracers. (Rohit Mathur, 919 541 1483; Jon Pleim, 919 541 1336)

Final updates have been applied to the air quality forecasting version of CMAQ (CMAQ-F) for running tests with aerosols at the National Weather Service's National Centers for Environmental Prediction on an eastern United States domain roughly three times the size of the current northeast domain that is running operationally. In addition to updating the code to correspond to the latest updates in the version of CMAQ scheduled to be released in August, modifications were made to allow for aerosol optical depth calculations from the output visibility file. (Jeffrey Young, 919 541 3929)

11. Community Multiscale Air Quality (CMAQ) Model for Air Toxics. A comparison was made between predictions from two different models for the annual averages of five Hazardous Air Pollutants (HAPs): formaldehyde, acetaldehyde, 1,3-butadiene, benzene, and perchloroethylene. Predictions came from the Community Multiscale Air Quality (CMAQ) and Assessment System for Population Exposure Nationwide (ASPEN) models. The latter model supports National Air Toxics Assessments by the U.S. Environmental Protection Agency. CMAQ predictions were based on simulations for 2001 and used a grid cell resolution of 36 x 36 km^2. CMAQ predictions are within a factor of two of the observations for formaldehyde and acetaldehyde. (William T. Hutzell, 919 541 3425)

12. Fire-related Emissions in CMAQ. University of Maryland MODerate Resolution Imaging Spectro-radiometer (NASA/MODIS) Rapid Response daily fire pixel data have been obtained and processed to identify the location and time period of major fire events for 2001. The Community Multiscale Air Quality (CMAQ) modeling domain for 2001 covers the continental United States with a 36-km grid resolution. Using the MODIS data, fire-related emissions are being reallocated in space and time to improve the original emissions estimates that had a very coarse resolution of monthly and state-level descriptions. CMAQ simulations will be repeated with these refined emission estimates to see if it results in improved $PM_{2.5}$ predictions during major fire episodes in August and May 2001. A paper will be presented at the upcoming Community Modeling and Analysis System (CMAS) workshop in October 2004, and a manuscript will then be prepared for the *Atmospheric Environment* special issue on model evaluation. (Dev Roy, 919 541 5338; Alice Gilliland, 919 541 0347)

The integration of parts of BlueSky into the Sparse Matrix Operational Kernel Emissions (SMOKE) modeling system is proceeding. BlueSky is a modeling framework designed to predict cumulative impacts of smoke from forest, agricultural, and range fires, while SMOKE is the emissions processing system used with air quality models like CMAQ. During July, work focused on building the plume rise algorithm to be used with wildfires. BlueSky computes emission estimates based on the fuel loadings for specific wildfire events. SMOKE is being updated to read output from BlueSky and to calculate the plume rise from wildfires using a layer-by-layer approach dependent on hourly meteorology. Using a single large wildfire as a test case from August 2001 in Washington State, plume rise has been calculated on a hourly basis for the duration of the fire. A prototype plume rise module for fires (LAYFIRE) has been tested for this specific case. Future work includes testing of the module with a large emission inventory for an entire state during a single month in 2001. Additional work to be done is to fully design and implement a method of bringing fire activity data into the BlueSky-adapted

framework and to connect the output from BlueSky with SMOKE in a robust efficient method. (George Pouliot, 919 541 5475).

13. The Air Quality Center of Excellence Pilot. The New York State Department of Environmental Conservation (NYSDEC) has now successfully used the EPA's National Environmental Scientific Computing Center (NESCC) IBM eServer Cluster 1600 "emerald" to run preprocessing programs for air quality forecasting simulations and data reduction. NYSDEC has also performed Community Multiscale Air Quality (CMAQ) runs on EPA's compute and data grid and transferred daily data archives to EPA's science ftp server. Efforts to develop and implement information technology tools to facilitate the NYSDEC collaboration have proven successful. (Gary Walter, 919 541 0573)

14. Micrometeorology and Pollution Transport Within Urban Building Environments. Much is being learned about how best to set up computational fluid dynamics (CFD) simulations to support environmental simulations and the issues that most affect comparability with both physical model studies and field measurement studies. The choice of boundary conditions, grid resolution and structure, and turbulence models significantly affect the outcome of a solution. Transport and dispersion can be well simulated for flat plate boundary layers as used in physical model studies. Transport and dispersion simulations are more complicated for atmospheric flows due to the complex temporal-spatial wind fluctuations. During July, a major improvement in the method to generate working meshed volumes for a complex model domain like Lower Manhattan was developed. This improved method provides the ability for accelerated development of applications and will make it easier to expand the present study area in Lower Manhattan. To date, the project has focused on CFD applications using Reynold's-average Navier-Stokes (RANS) steady-state solutions and the standard k-e turbulence models. This is being extended to include unsteady solutions and higher order turbulence models. This research will be helped by using the multiprocessor cluster at Department of Energy's Argonne National Laboratory, which was started during July following the installation of the Fluent CFD code. Detailed technical papers will be prepared as this project reaches significant conclusions. (Alan H Huber, 919 541 1338).

15. CMAS 2004 Workshop – Special Session on Model Evaluation. The Community Modeling and Analysis System (CMAS) center at the University of North Carolina at Chapel Hill, Carolina Environmental Program, will be sponsoring the 3rd annual Models-3 Users' Workshop, October 18-20, 2004, at the Friday Center at the University of North Carolina at Chapel Hill. Air quality model evaluation is the special focus of this workshop. An announcement and preliminary agenda are available at http://www.cmascenter.org. About 35 of the approximately 90 papers submitted will be in the Model Evaluation Session. Papers from this session will be submitted for consideration to *Atmospheric Environment* for publication in a special issue in late 2005. Extended abstracts and presentations from other sessions will be published on-line through the CMAS web site. The workshop will be held immediately prior to an intercontinental transport air quality workshop being sponsored by the U.S. EPA Office of Air Quality Planning and Standards. (Bill Benjey, 919 541 0821)

Idaho Falls

16. Smart Balloon Launches During NEAQS - ITCT. During the month of July, two smart balloons equipped with ozone analyzers were launched in Lagrangian experiments as a part of the New England Air Quality Study - Intercontinental Transport and Chemical Transformation (NEAQS-ITCT). The low-power ozone analyzers were developed over the past year at the University of New Hampshire (Robert Talbot and Don Troop) and we then integrated them into our smart balloon instrument package. The smart balloons were used not only to track and measure ozone in the plume of pollution moving over the northeastern tip of Long Island, but also were used as a marker for the NOAA P-3 aircraft to return to the same plume for additional air quality sampling repeatedly over extended periods of time.

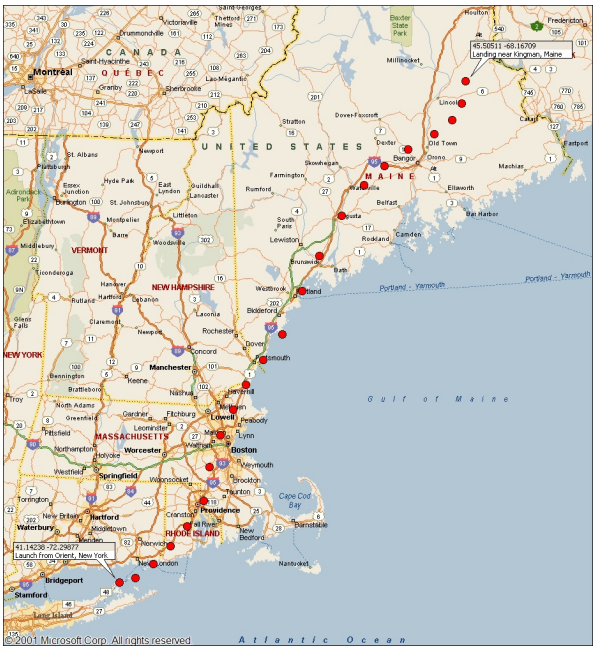

Figure 1. Smart balloon #1 launched from Orient, NY and recovered near Kingman, ME after a 21- hour flight. Red dots show the path of the balloon at 1 hour intervals.

On July 15th, Balloon #1 was launched from the Orient, New York, fire station and tracked for 21 hours. The flight was terminated near Kingman, Maine. The balloon was recovered in the very dense forest of northeastern Maine, nearly two days after it was launched. Recovery of Balloon #1 would eventually allow us to launch a fourth balloon later in the experiment (See August Report). Position, altitude and ozone data were recorded and stored every ten seconds over the full period of time. Altitude control worked very well except for a short period of time north of Boston when the balloon encountered a rain storm. The sudden afternoon rain caused the balloon to descend from around 600 meters ASL level to below 100 meters ASL.

On July 20th, Balloon #2 was launched from the Orient fire station and tracked for 49 hours. The balloon flight was terminated five miles north of Prince Edward Island, Canada, when a rapid decrease in helium pressure was detected. A possible cause for the sudden decrease in helium pressure could have been a substantial leak in the cut down valve at the top of the balloon. The NOAA P-3 aircraft was able to return three times to the air parcel marked by Balloon #2 over its 49-hour flight. (Randy Johnson, 208 526-2129, and Shane Beard)

Figure 2. Balloon #2 launched from Orient, NY on July 20, 2004 and terminated 5 miles north of Prince Edward Island, Canada. Red dots show the path of the balloon at one hour intervals.

17. Pentagon Shield. The data from the ARL Programmable Integrating Gas Samplers (PIGS) are undergoing a through quality control review. We

have completed a comparison of field records and analysis records to ensure that the correct data is associated with each field location. A time history plot of each sampler was created and reviewed for consistency within the 12-bag sample set and with nearby samples. Any apparent problems were investigated carefully and the data appropriately flagged if there were indications that it was unreliable. The data have also been compared with the list of locations used in each Intensive Observation Period (IOP) to make sure that data is available for each location. A description of the locations is being generated to be delivered with the data set.

Initial analysis, calibration and peak extraction from the continuous analyzer data has been completed. The results of this process have been verified by a second analyst. An algorithm to extract the data and estimate the baseline from the ultra pure air ran as calibration gas has been implemented and appears to provide reasonable results. Generation of output files that are correctly adjusted for baseline drift and that contain QC flags is currently in process. These files will need to be reviewed and any errors corrected before they may be released. Correct location information will also be included. (Roger Carter, 208 526-2745, and Debbie LaCroix)

18. CBLAST-High. Final preparations were completed for the upcoming hurricane season. Data were processed from last month's NOAA P-3 test flights in Tampa. The data confirm that each of the BAT instruments operated properly. The P-3 aircraft was unavailable for hurricane research flight in July because of its participation in the NAME project. The P-3 is due to return to MacDill Air Force Base in early August and is scheduled to be available for CBLAST tasking by August 18. The CBLAST Hurricane project will be transferred to NOAA Atmospheric Turbulence and Diffusion Division in Oak Ridge effective August 8. Further developments in the CBLAST-Hurricane project will be reported by ATDD. (Jeff French, 208-526-0566)

19. Extreme Turbulence Sphere. Much of the testing of the modified "big port" ET sphere has been completed. Work is now focusing mostly on preparations for deployment. This system has performed reliably in pre-deployment tests, and appears to handle rain without serious problems. ATDD is still working on an alternative sphere design that uses a pump to backflush the pressure ports. There were no conclusive results reported on this alternative system as of the end of July. Currently, the plan is to deploy three ET spheres. Two of these will definitely be the big-port design. The third will be the backflushed sphere if testing shows that it works properly. (Richard Eckman, 208 526-2740, and Tom Strong, FRD; Ron Dobosy and Dave Senn, ATDD)

20. Proteus Aircraft. Work on the fabrication of a BAT probe for the Proteus aircraft was completed in July. Final bench testing and calibration were also completed. Installation and integration of the system were originally due to begin in July/August but has been postponed until fall after the aircraft returns from a deployment in Alaska. (Jeff French, 208-526-0566)

21. Idaho Mesonet Semi-Annual Preventative Maintenance and Calibration. The semi-annual preventative maintenance and calibration of all meteorological sensors in the INEEL Mesonet that was started in June was completed during the month. During the inspection, all of the meteorological instrumentation on the 35 towers were examined to verify proper operation and calibration. Necessary repairs or replacements were made to ensure continued operation. All instruments were calibrated to NIST-traceable standards to verify that the data being collected are accurate and complete. (Tom Strong, 209 526 5434)

As a part of its Idaho mesonet, FRD has been operating a surface-flux tower at INEEL for several years, but some of the equipment has started to deteriorate. In particular, sensors associated with computing the soil heat flux appear to have malfunctioned. New sensors have been purchased, including some spares that will allow rapid replacement of malfunctioning sensors in the future. FRD is also planning to purchase some Li-Cor 7500 open-path H_2O and CO_2 analyzers as replacements for the aging Infrared Gas Analyzer (IRGA) currently in use with the flux tower. This tower is expected to see increased use at the INEEL for estimating atmospheric stability, mixing depth, and turbulence levels. At some point, a second flux system may be installed at the northern end of INEEL, since the dispersion meteorology there is often substantially different from the southern end. (Richard Eckman, 208 526 2740, Tom Strong, Kirk Clawson)

22. INEEL Mesoscale Modeling. The malfunction of FRD's main web server disrupted the public interface to the FRD mesoscale forecasts. This hiatus was used to perform several upgrades to the model. It is now clear that the soil volumetric water content provided by the NCEP Eta model is almost always too high for Southeast Idaho. This leads to unrealistic surface energy budgets, particularly for the sagebrush-steppe ecosystem around the INEEL. The mesoscale model configuration has been changed to use the Pleim-Xiu land surface scheme, because it allows one to specify more realistic soil water contents for each land-use category. It also allows the soil water to be nudged based on surface temperature and humidity observations. The new configuration provides much more realistic surface energy budgets, and it also appears to do a better job of forecasting peak afternoon wind speeds. (Richard Eckman, 208 522 2740)

Las Vegas

23. Department of Energy (DOE) Meteorological Coordinating Council (DMCC). ARL chairs the DOE/DMCC. Preliminary planning for the 10th anniversary meeting of the DMCC in November has begun. This meeting will be held in the Forrestal Building in Washington, D.C. on November 18-19. (Darryl Randerson, 702 295 1231, and Walt Schalk, 702 295 1262)

A revision of the dispersion "bible" (Atmospheric Science and Power Production) is being contemplated. A draft outline has been prepared of potential chapters in a new technical document being proposed for DOE and NNSA. The new work is being designed to update the earlier work, which was published in 1984. The proposed title for the new book is Atmospheric Sciences and Releases of Hazardous Materials. (Darryl Randerson, 702 295 1231)

24. North American Monsoon Experiment (NAME). SORD personnel participated in the NOAA NAME Project by collecting 52 upper-air soundings from the Desert Rock Meteorological Observatory (DRA) and 8 soundings from the Nevada Support Facility (NSF). These data were promptly compiled and transmitted to the NAME Forecast and Research Center in Tucson, AZ. The data collected on July 14 were just prior to and during a "Gulf Surge". A marked moisture gradient was measured between DRA and the NSF on July 14. (Darryl Randerson, 702 295 1231)

25. NOAA Cooperative Institute for Atmospheric and Terrestrial Applications (CIASTA). Mesoscale Modeling - NV-RAMS ran to completion on the University of Nevada-Las Vegas (UNLV) computer system 28 of 31 days (90% completion factor). The UNLV computer system was down for several days for repairs/upgrades. Data are continuing to be saved daily, and backed up to CD monthly (3 CDs).

The 12z model run is continuing to work consistently. This activity is likely to be critical to the emerging studies of air pollution in the Las Vegas valley, led by CIASTA. (Walt Schalk, 702 295 1262)

26. New Geographic Information System (GIS) Backgrounds. New terrain backgrounds have been generated for the NTS and Southern Nevada utilizing U.S. Geological Survey Digital Elevation Model data with a resolution of 10 meters. These data files are in a GIS graphic format that requires special software to view them. A program named "DLGV32" was downloaded that reads and displays these files. The program allows the displayed information (in a pseudo 3D form) to be saved as an external JPG type file (other formats are also available). These new graphics can then be utilized as backgrounds for plotting--displaying the NTS boundaries, special locations, etc. (Doug Soule', 702 295 1266)