NOAA Air Resources Laboratory
Quarterly Activity Report

(January – March 2008)

Contents

32. ***WRF Mesoscale Model***
33. ***Federal Emergency Response Organization Support***
34. ***American Nuclear Society***
35. ***Air Permit Modeling***
36. ***GoggleEarth***
37. ***Compliance Data***
38. ***Extreme Weather***

Highlights

1. WMO Sponsored Source-Attribution Experiment. A WMO sponsored source-attribution test was conducted for a simulated measurement event that occurred between February 29 and March 2, 2008. Participating centers included NOAA, the UK Met Office, China, and Australia. A report was prepared in which the individual center predictions of the source-receptor-sensitivity function were reformatted into a graphic that showed the most probable source location for measurement data. roland.draxler@noaa.gov

2. United Nations Environment Program Report on Mercury Air Transport and Fate Research. A Division scientist assisted in the development of a report coordinated by the United Nations Environment Program (UNEP) Global Partnership on Mercury Air Transport and Fate Research. This report, entitled the UNEP Mercury Transport and Fate Report (T&F Report) is a step forward from the UNEP 2002 Global Mercury Assessment report and from the synthesis papers prepared by five expert panels at the last International Conference as a Global Pollutant (ICMGP) held in Madison, USA in August 2006, which have been published in *Ambio* (February 2007) by the Royal Swedish Academy of Science. As a member of the ICMGP expert panel on "Attributing Sources of Mercury Deposition," the Division scientist was asked to be lead author on a chapter of the T&F Report regarding the importance of intercontinental transport on regional mercury modeling. An initial draft of the T&F Report will be composed at a meeting beginning April 7-11, 2008 in Rome, Italy, in coordination with the United Nations Economic Commission for Europe convention on Long-Range Transport of Air Pollution. o.russell.bullock@noaa.gov

3. Carbon Monitoring Workshop. A workshop, including 20 participants from all over the country, was hosted by Marc Pitchford. The topic for discussion was carbonaceous particulate matter (PM) monitoring issues facing the IMPROVE (~170 site remote-area monitoring network) and Chemical Speciation Network (~220 urban monitoring sites) programs. Carbonaceous PM is one of the most abundant components of PM and is responsible for health, visibility and climate effects. It is composed of a mixture of thousands of individual organic compounds, there are no standard reference materials nor any reference analytical methods, and collection of quartz fiber filters (required for compatibility with the thermal-optical analysis methods employed) are plagued by sampling artifacts. Modest changes to the monitoring/analysis procedures have been shown to produce discontinuities in the data record from both networks. The two-day workshop was held at the University of California-Davis from January 22 to 24 and resulted in significant proposed changes to both programs as well as a series of special studies that should provide better quality and comparability of carbon PM data from these two national monitoring programs. marc.pitchford@noaa.gov

Air Resources Laboratory – Headquarters

4. National Mercury Monitoring Network. Mark Cohen participated in multiple conference calls and meetings related to the development of a national mercury monitoring network. He reviewed documents and offered substantial feedback and analyzed, developed and presented a prioritized list of potential intensive mercury monitoring sites at a critical March 4, 2008 meeting. In addition, Mark prepared and presented detailed siting criteria with particular attention to locating sites that were useful for atmospheric model evaluation. Mark also worked with colleagues at the Grand Bay NERR, the Canaan Valley Institute, and Beltsville to develop handouts and other information about NOAA-related potential intensive mercury monitoring sites. The current phase of this organizing effort is leading toward a May 5-7 National Mercury Monitoring Workshop in Annapolis MD. mark.cohen@noaa.gov (with Richard Artz and Winston Luke).

5. Global Eulerian Model. Mark Cohen began working with a global Eulerian model developed by Roland Draxler. Preliminary work has involved initial attempts to add capability to simulate multiple chemical species, atmospheric deposition, and atmospheric chemistry. Also, substantial work was done analyzing, assembling, and parsing 2002 National Emissions Inventory mercury emissions inventory data and comparable data from Environment Canada. Data from Environment Canada had been requested for years and a complete dataset for the year 2000 was finally obtained and analyzed. Maps have been prepared and the dataset has been shared with the EPA. mark.cohen@noaa.gov

6. Smoke Forecast Update. Roland Draxler began testing updates to the smoke forecasting system which includes the following modifications: velocity divergence for vertical motion, revised mixed layer depth algorithm, removed plume rise restrictions, added CO and non-methane hydrocarbons (NMHC) to particle, reduced aggregation grid from 0.2 to 0.1 degrees, modified PARDUMP (particle dump) to output hourly for CMAQ boundary conditions, and started independent forecasts for Alaska and Hawaii. roland.draxler@noaa.gov

7. February HYSPLIT Update. A generic Postscript color fill program was created to show values on a global concentration grid. The program also works with regional grids. The standard concentration plotting program had difficulty with global grids. The concentration probability programs were revised to output values consistent with a typical frequency box plot. A box plot routine was added to the ensemble display menu. A testing script was created to check out the executables created from a UNIX compilation. The temporal emissions file program was modified to permit multiple species to reside on the same particle when the mass dimension namelist variable was set to a value equal to the number of pollutant species. The minimum particle emission rate was set to one per processor, when the model is run in a multi-processor environment. The puff split-merge algorithm was improved to avoid the situation during very long-duration simulations when the number of puffs reaches the array limits cause further splitting to shutdown while puff growth continues. In this revised version, the onset of splitting is delayed and the merging parameters are relaxed to permit more distant puffs to merge. roland.draxler@noaa.gov

8. QWIK Code and User Guide Update. The HYSPLIT-QWIK interface was updated to be able to access the new NAM-12 CONUS tiles especially designed for emergency response applications. There were several significant modifications to the script to be able to automatically select the appropriate tile based upon the starting location. roland.draxler@noaa.gov

9. Developmental Smoke Forecast Update. The results of last year's research on improving the wild fire smoke forecast predictions were applied to the developmental run so that performance statistics can be computed and compared with the current operational run. If significant improvements are noted by the end of this summer's fire season, the changes will be incorporated into the operational model. The primary modifications are restrictions on the plume rise height based upon fire duration, a reduction in the fire location aggregation grid from 0.2 to 0.05 degrees, increased maximum smoke age from 72 to 96 h, and permitted short-duration emissions south of 23N to emit into the forecast period. Other changes that will not affect the performance statistics include adding two additional species (CO and NMHC) and output of the particle positions each hour into the forecast period to permit their use in creating a boundary condition file for CMAQ. roland.draxler@noaa.gov

10. Progress on Manuscript. A paper entitled "Comparison of Radiosonde and GCM Vertical Temperature Trend Profiles: Effects of Dataset Choice and Data Homogenization" by John Lanzante and Melissa Free was accepted by the Journal of Climate in March. melissa.free@noaa.gov

11. Workshop on the Applications of GPS Radio Occultation to Climate. Dian Seidel, along with colleagues from NOAA NESDIS (Headquarters, STAR and NCDC) and from the NOAA Climate Program Office, participated in this workshop held at UCAR in Boulder, CO on March 17-18. The workshop brought together members of the NOAA climate science community and the Global Positioning System Radio Occultation (GPS-RO) community, to explore ways in which atmospheric observations based on GPS-RO principles might be useful in climate research and monitoring. NOAA is considering supporting future operational GPS-RO observations, and the main focus of the workshop was to clearly identify the potential benefits of GPS-RO data for climate. Participating NOAA climate scientists are providing input to NESDIS program managers developing budget alternatives related to GPS-RO. dian.seidel@noaa.gov

12. GCOS (Global Climate Observing System) Reference Upper Air Network. The GCOS Reference Upper Air Network (GRUAN) has been initiated. The network is meant to provide ground-based reference atmospheric profile observations of meteorological and atmospheric composition parameters to meet climate requirements. Working with GCOS, NOAA scientists have been advocating the establishment of such a network for several years and previously hosted two planning workshops to define observational requirements and evaluate instrument options. In February, Dian Seidel and other NOAA colleagues participated in two meetings, held at the Richard Assmann Observatory in Lindenberg, Germany, which has been designated by GCOS as the GRUAN Lead Center. The meetings were: 1) the GCOS Working Group on Atmospheric Reference Observations (Feb 25); and 2) the GRUAN Initiation Meeting (Feb 26-28). Topics included potential GRUAN sites, instrumentation and launch schedules; data management and quality control; coordination of GRUAN with other programs; and development of an action plan for GRUAN. Additional information about the workshop is available at http://metportal.dwd.de/mol (click on GRUAN). dian.seidel@noaa.gov

13. American Meteorological Society Annual Meeting. Dian Seidel participated in the following activities at the AMS Annual Meeting in New Orleans (January 20-24): participated in AMS Council meeting, presented a paper in Conference on Climate Variability and Change, helped organize Town Hall meeting on new AMS Green Meetings initiative, completed oral examination

for AMS Certified Consulting Meteorologist program. dian.seidel@noaa.gov

14. Outreach. Dian Seidel was involved in multiple outreach activities at local area schools in March.

15. HYSPLIT Package Upgrade at NCEP. The NCEP Senior Duty Meteorologist (SDM) runs HYSPLIT for volcanic ash, radiological, or other dispersion events and exercises. The SDM runs a setup script to configure the model inputs and subsequent scripts execute HYSPLIT and the post-processing. In response to a request from NCEP, a test script was developed to test the operational scripts for a series of "typical" dispersion runs.

Final testing in preparation for submitting the upgrade to NCEP is currently in progress. barbara.stunder@noaa.gov

16. Volcanic Ash Dispersion Modeling. An inter-agency effort between meteorologists and volcanologists to improve eruption source parameters is in progress. A modeling sub-group is evaluating the effect of ash particle size distribution and vertical distribution in the initial eruption column. Several HYSPLIT runs have been provided for this. barbara.stunder@noaa.gov

17. Alaska and Hawaii Meteorological Grids for NCEP. The operational NCEP smoke runs use NCEP North American Model (NAM) meteorological output over the continental U.S. and surrounding areas and NCEP Global Forecast System (GFS) meteorological output over Alaska and Hawaii. Scripts were developed to create NAM grids over Alaska and Hawaii. As one of the steps leading to operational status, these scripts have been given to the NCEP Environmental Modeling Center for further testing. barbara.stunder@noaa.gov

Atmospheric Turbulence and Diffusion Division

18. Climate. The Climate Reference Network (USCRN) is approaching 120 sites with three new installations this quarter. Three new sites were also installed for the Historical Climate Network (HCN) in Alabama, giving a total of 14 HCN sites in that state. Twenty-three sites received annual maintenance visits, ensuring continued reliability and quality in the data stream. mark.e.hall@noaa.gov

19. Air Quality. Instrumentation is now installed to measure the primary terms of the mercury budget for the 900-acre Wymer Run watershed entirely contained on land owned by the Canaan Valley Institute in West Virginia. Assessment of mercury uptake by animals is planned. These data will support development of a mercury model for watersheds. steve.brooks@noaa.gov

20. Plume Dispersion. Rapid availability of wind and turbulence information to emergency responders is being addressed, drawing on new developments in both instruments and modeling. We are exploiting UrbaNet data from the National Capital Region to develop methods for quick estimates of wind and turbulence in a complex, but data-rich urban environment. In east Tennessee, the Weather Research and Forecast Model came into regular operation at ATDD. Forecasts are being archived to produce model output statistics with observations from our local mesoscale network, including vertical profiles from episodic RAWINsonde launches. will.pendergrass@noaa.gov

Atmospheric Sciences Modeling Division

21. Parameterization of Heterogeneous N2O5 Reaction Probability. Model results for wintertime particulate nitrate are sensitive to the heterogeneous reaction probability of dinitrogen pentoxide on particle surfaces (γ_{N2O5}). Last quarter, Division scientists published a new parameterization of γ_{N2O5} for particles containing sulfate, nitrate, and ammonium (Davis, Bhave, and Foley, ACPD, 7:16119-16153, 2007). The publication of this parameterization stirred up some debate regarding the dependence of γ_{N2O5} on relative humidity (RH) at RH > 50%. This quarter, further research was conducted on this topic including an extensive survey of laboratory measurements of γ_{N2O5} on various water-soluble substrates. An alternative parameterization of γ_{N2O5} has been developed and will be tested in the Community Multiscale Air Quality (CMAQ) model in preparation for the upcoming public release. Motivated by the results of our work, EPA scientists approached Division scientists to plan a set of laboratory experiments aimed at improving the parameterization of γ_{N2O5} in future versions of the CMAQ model. prakash.bhave@noaa.gov, kristen.foley@noaa.gov

22. Secondary Organic Aerosol Module Upgrade. Division scientists made a major upgrade to the Community Multiscale Air Quality (CMAQ) model treatment of secondary organic aerosol (SOA) species. During this quarter, several test simulations were conducted in preparation for the upcoming public release of the CMAQ model. Model simulations of summer 2003, January 2006, and August 2006, have been conducted using the newly developed SOA module and the previous SOA module. Preliminary results suggest that predictions using the new SOA module exhibit better seasonal and spatial patterns for aromatic and biogenic SOA and predictions of total carbon exhibit a diurnal profile that is consistent with observations. Model results are being evaluated against source-specific organic carbon measurements in Research Triangle Park and semi-continuous organic and elemental carbon measurements in Duke Forest. Work is also underway to better couple global and regional air quality models by developing boundary conditions for CMAQ using Goddard Earth Observing System chemistry predictions. Well-defined boundaries in both time and space are important for some of the new SOA species, which have precursors with long chemical lifetimes. annmarie.carlton@noaa.gov, Sergey Napelenok, and Prakash Bhave

23. Air Quality Model Evaluation International Initiative. Following on a successful workshop in August 2007 covering the evaluation of regional-scale numerical air quality modeling systems in North America, a Steering Committee has been formed to explore the possibility of holding a similar Workshop in Europe to extend the discussions to an international audience, and compare and contrast evaluation techniques on both continents. The Steering Committee is composed of about 20 members from modeling organizations in Europe, U.S., and Canada. st.rao@noaa.gov, kenneth.schere@noaa.gov

24. Regional Air Quality Model Evaluation Report. A Workshop on the evaluation of regional-scale air quality modeling systems was held during August 7-8, 2007 in Research Triangle Park, NC, sponsored by the American Meteorological Society and the U.S. EPA, and was attended by over 90 members of the air quality modeling community. Some of the ideas discussed at the Workshop are being captured in a manuscript developed by members of the Workshop's Steering Committee. A framework for model evaluation is presented, composed of several perspectives on model evaluation including operational (are we getting the right answers), diagnostic (are we getting the right answers for the right reasons), dynamic (does the model correctly simulate changes due to emissions and meteorology), and probabilistic (what is our confidence in the model predictions). New evaluation

techniques for regional scale models are emphasized, and modeling uncertainty is explored through the use of ensemble and Bayesian methods. The Steering Committee hopes to complete the draft manuscript and submit for review by summer 2008. The model evaluation framework presented here has also been embraced by the Steering Committee for the new Air Quality Model Evaluation International Initiative, a joint European, U.S., and Canadian project. kenneth.schere@noaa.gov

25. Air Quality Forecast Model Development and Testing. In preparation for the 2008 implementation of the National Air Quality Forecast Guidance system, a number of upgrades to both, the Community Multiscale Air Quality (CMAQ) model and a pre-processor for CMAQ (PREMAQ) code configurations, as well as input emission data sets were tested. The interface processor, PREMAQ, was updated to include an alternate formulation of the aerodynamic resistance term used in estimation of dry deposition velocities, modifications to speciate emission data sets compatible with both the CBM-IV and the updated CB-05 chemical mechanisms, and to accommodate data sets with alternate mobile emissions estimates. The CMAQ code was updated to include the CB05 chemical mechanism. A number of simulations over a retrospective period in 2007 were performed to test various changes in the modeling system and included testing of:

- Impact of updates to the North American Mesoscale (NAM) model on CMAQ predictions of O_3.
- Impact of emission updates (estimates used in 2007 forecasting and updates based on the 2005 National Emissions Inventory and a 2009 projected inventory) on forecast performance
- Impact of alternate chemical mechanisms (CBM-IV and CB-05) on O_3 forecasts with the system
- Impacts of changes in method for estimation of dry-deposition velocity on O_3 predictions.

Changes were also incorporated in the CMAQ input/output structure to facilitate the application of the model on a 60-layer configuration that exactly matches the layer configuration employed in the driving NAM model. Simulations with this CMAQ configuration will be used to assess the impacts of using a reduced layer structure in operations. Efforts were also devoted towards improving the representation of O_3 in the free troposphere. The stratospheric influence on O_3 was parameterized by enforcing the condition of proportionality to Potential Vorticity (PV) in the top CMAQ layer (~100 mb); spatially and temporally varying PV fields were estimated from the NAM fields. Extensive comparisons of resultant simulated profiles with measurements from the ozonesonde launches during the 2006 Texas Field Study indicated improved representation of simulated O_3 vertical structure. The approach is being further refined to include a PV-based scaling for specification of lateral boundary conditions as well as in developing a more robust constant of proportionality. rohit.mathur@noaa.gov, George Pouliot, Jonathon Pleim, Jeff Young, and David Wong

Field Research Division

26. Perfluorocarbon Tracer (PFT) Analysis Development. Final testing of the bag cleaning protocol developed for the 3-PFT method was completed in early January. These tests confirmed that the protocol was effective in cleaning bags with long term exposure to high concentrations down to below the detection limit for each species. This concluded all testing of the PFT method and the method is at a stage where it is ready for actual experimental work. A final report summarizing the method, procedures, protocols, and cautionary notes was prepared. Key points from this document were summarized in the last quarterly report. dennis.finn@noaa.gov

27. Fast Response Tracer Analyzer Data System Upgrade. A new data system for our existing fast response tracer analyzers is being developed. It will be based on an embedded microcontroller and will store data on a compact flash card. A prototype system is running and the debugging of the firmware and hardware interfaces is nearly complete. A printed circuit board layout for the system is being created and should be completed soon. Hopefully, an order for printed circuit boards can be placed in the next few weeks. roger.carter@noaa.gov

28. Low Cost Tracer Detector and Existing Equipment Upgrade. FRD staff have been studying the feasibility of creating a low-cost version of the fast response analyzers. The current systems are too expensive for deployments in larger numbers, and a lower cost version would offer a broader range of potential applications. There is no guarantee that a low-cost system can be developed, so this effort is more in the line of high-risk, high-payoff research. Part of this effort has been the development of a new low-cost SF_6 detector that can measure concentration fluctuations. When the current prototype detector is used with the oxygen removal system of the existing fast response analyzers, it measures SF_6 with a detection limit of about 200 ppt and a response time of about 10 seconds. Although this performance is significantly worse than the current fast response analyzers, it is nevertheless usable in many experiments and it will be far less costly to build and deploy.

New oxygen removal systems and improvements to the existing oxygen removal system are also being investigated. Experiments with a solid state oxygen removal system showed that it was impractical for use in an analyzer. An electrolyzer that generates hydrogen from distilled water has also been tested. This has the potential of replacing the compressed hydrogen tank used in the current system, making the system safer to operate. One of our current fast response tracer analyzers was successfully run with hydrogen generated by the electrolyzer and with a low cost detector, demonstrating that it would be possible to build a tracer analyzer that does not require tanks of compressed hydrogen. However, interfacing the electrolyzer with the analyzers will be a challenge to develop, because the hydrogen must be supplied under controlled and constant pressure. roger.carter@noaa.gov

29. Las Vegas Roadway Toxics Tracer Study. FRD is continuing to work with ASMD and EPA on conducting a roadway tracer study later this year. However, questions have arisen regarding the suitability of the presumed study location on Interstate 15 in Las Vegas. The site was originally an open field but is now a fenced parking lot for trucks. Prevailing wind directions are also problematic. One option being pursued is to conduct a more effective study the Idaho Falls area. Part of the study's focus is on the effects of large sound barriers on near-road dispersion. Idaho Falls does have one road with such a sound barrier, but it has also been suggested that a temporary barrier could be constructed at INL or another location and allow much better control over the setup of the study. It appears that an effective barrier could be constructed Lego-block style using large 900 kg straw bales. Such bales are inexpensive and easy to obtain in the Idaho Falls area. kirk.clawson@noaa.gov

Special Operations and Research Division

30. ACCENT Workshop and WMO-SAG Precipitation Chemistry Meeting. Marc Pitchford represented the IMPROVE Network at the ACCENT (Atmospheric Composition Change European Networks of Excellence) Workshop on Network Harmonization and Data Intercomparability, and was the local host for the annual WMO-Science Advisory Group on Precipitation Chemistry meeting

held in Las Vegas, NV (January 28 through January 31). The two gathering with overlapping participants brought together managers of air quality monitoring networks from Europe, Africa, Asia, and North America (both the U.S. & Canada) to discuss data quality and comparability (ACCENT) and to continue work on an updated global trends report (WMO-SAG). marc.pitchford@noaa.gov

31. Consequence Assessment. Walt Schalk continued training on the Department of Energy (DOE), National Nuclear Security Administration (NNSA), National Security Technologies, LLC, consequence assessment procedures and methods for the Nevada Site Office (NSO) and Nevada Test Site (NTS). The training included radiological and chemical scenarios that require event classification, protective action recommendations, dispersion model predictions, and graphical product development for health physicists, industrial hygienists, incident commanders, safety advisors, and emergency managers. Participation in the emergency response quarterly drill presented an assessment on training to date. In addition, participation in several preparatory meetings and tabletop drills aided preparation for a full participation exercise to be held in April 2008. walter.w.schalk@noaa.gov

32. WRF Mesoscale Model. Statistics are being collected for the Las Vegas/NTS WRF runs. This information will be used to provide feedback into the model. Numerous compiler, model, and output routine errors were fixed. Work continues to improve the low-level sounding and stability characteristics of the model in the lower dry lake beds of the NTS. kip.smith@noaa.gov

33. Federal Emergency Response Organization Support. In January Walt Schalk attended the FRMAC Transition meeting at the Las Vegas Environmental Protection Agency (EPA) office. The meeting discussed issues relating to the transitioning of the Federal Radiological Monitoring and Assessment Center and an initial characterizing phase during a national response event from the DOE to the EPA for final characterization and restoration phase. NOAA's role is small, and this meeting dealt with higher level issues. Our role would be setting up/securing local WFO meteorology support and/or leaving or installing meteorological observation towers for a full set of data to complement the concentration. walter.w.schalk@noaa.gov

34. American Nuclear Society. In March**,** Walt Schalk attended the American Nuclear Society Topical Meeting on Emergency Response, and chaired a session on Severe Weather Planning for Key Facilities in which two SORD presentations were given. The topics were: "Investigation of Range-Applicable Lightning Detection Systems," and "Nevada Test Site Lightning and Hazardous Weather Detection and Protection Orders". In addition, a presentation was given in the Software Quality Assurance for Emergency Preparedness and Response session titled, "The DOE Meteorological Coordinating Council (DMCC) Perspective on the Application to Meteorological Software of DOE's Software Quality Assurance (SQA) Requirements." walter.w.schalk@noaa.gov

35. Air Permit Modeling. Work was begun to provide air permit modeling support to NNSA/NSO for the NTS. The American Meteorological Society (AMS)/EPA Regulatory Model Improvement Committee (AERMIC) Model (AERMOD) was installed on SORD computers. Weather data from the NTS meso-net was compiled and processed for 2007. SORD is working with NTS contract staff to gather input source term information. kip.smith@noaa.gov

36. GoogleEarth. A first draft of the capability to display the SORD MEteorlogical Data Acquisition Mesonet (MEDA) wind data on Google Earth was completed. Wind vectors are

displayed over the NTS satellite picture background in three colors; one of which corresponds with High Wind Warning criteria. james.sanders@noaa.gov

37. Compliance Data. The 2007 data from 8 SORD MEDA meso-net towers were retrieved, compiled and analyzed. Data were processed into STability ARray (STAR) format (wind direction and stability class binning) for use by the NNSA/NSO NTS contractor to comply with the Clean Air Act, National Emission Standards for Hazardous Air Pollutants (NESHAPS) and provide appropriate documentation. walter.w.schalk@noaa.gov

38. Extreme Weather. The current Winter/Spring 2007-2008 season has been an extremely windy one for the NTS. Of special note was a high wind event on February 13th. Two stations (one on the southwest NTS, and the other in the central NTS) reported wind gusts of 127 and 114 miles per hour (mph). Five other stations reported over 90 mph gusts, and eight others over 80 mph. The maximum 15-min average wind was 90 mph. These winds exceeded the previous high wind event day, Tax Day 2002. walter.w.schalk@noaa.gov