

NOAA ARL Monthly Activity Report



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Highlights

1. Urban Dispersion Study. Preparation has begun for the NOAA Twin Otter's involvement in Joint Urban 2003, to be conducted in Oklahoma City, June - July 2003. Equipment installation will be in Tampa, FL 30 June - 4 July, with deployment to OKC on 7 July. The Otter is scheduled to fly approximately 25 hours. We will be conducting flux measurements, as well as measuring CO_2 and H_2O vapor (IRGA) and the state parameters. We will also be testing a new GPS system, the Garmin 16. GPS data will be compared with the Novatel data we currently acquire. gunter@atdd.noaa.gov, McMillen

Assembly and testing of ATDD's tower-based systems for Joint Urban 2003 are nearing completion. ATDD will provide three surface energy budget stations and two 30m crank-up towers, each with four levels of 3-D sonic anemometry and temperature. The new hardware collects four independent channels of sonic data via a USB port into a midget computer running Linux. Data are written to an internal hard disk, and then exported daily to a Zip drive, for collection by a "circuit rider". white@atdd.noaa.gov, Dumas, Heuer, Ludwig, and Meyers

Defense Research and Development Canada (DRDC) - Suffield hosted an Urban Dispersion Model Working Group meeting at the Canadian Forces Base in Suffield, Alberta, on May 13-14. Participants included representatives from Australia, Canada, the UK, and the US. Updates on progress in urban dispersion modeling at various scales were provided. An ATDD scientist provided an overview of the upcoming Joint Urban 2003 study in Oklahoma City, and a summary of the wind tunnel modeling of Oklahoma City that is still under way at the University of Hamburg. <u>hosker@atdd.noaa.gov</u>

The ATDD microbarograph array will be deployed in the Joint Urban 2003 study. Three new microbarograph sensors have been completed, and testing is underway. <u>auble@atdd.noaa.gov</u>, Nappo

2. *EPA and NOAA Join Forces to Study and Forecast Air Quality*. In a ceremony that took place on May 6, 2003, in Washington, DC, EPA Administrator Christine T. Whitman and Deputy Secretary of Commerce Dr. Samuel W. Bodman signed a Memorandum of Understanding (MOU), reaffirming their long-standing collaboration on atmospheric sciences research, and a Memorandum of Agreement (MOA) to develop and implement a national air quality forecasting system. The two agencies will join forces to enhance research in air quality modeling and atmospheric measurements for developing a consistent national numerical air quality model for short-term air quality forecasts for ozone, fine particulate matter, and visibility.

"An improved air quality forecast can mean a higher quality of life for many Americans, especially those most vulnerable to the effects of ozone air pollution. Air pollution control agencies across the country will use the new model that EPA and NOAA are developing to help people make better decisions to protect their health," said Dr. Bodman. "I am very pleased that EPA and NOAA have joined forces to advance local agencies" ability to forecast air quality," said EPA Administrator Whitman.

ARL is working closely with the National Center for Environmental Prediction of the National Weather Service in developing an integrated meteorological-chemical transport model for simulating ambient air quality over the continental United States as part of the MOA between NOAA and EPA. In the first phase of the forecasting project, EPA and NOAA will produce a numerical air quality model that provides daily forecasts for ozone in the northeastern United States by September 2004. Within five years, the system for ozone will deploy nationwide. The model is projected to be able to forecast particulate matter and provide a four day forecast within ten years. State and local air quality management agencies will continue to forecast local air quality, based in part upon the national air pollution concentration forecasts provided by the EPA-NOAA partnership. (S.T. Rao, 919 541 4541) **3.** *Atmospheric Mercury.* There is considerable attention being given to the transport and deposition of atmospheric mercury. Three ARL Divisions are directly involved – Silver Spring, Research Triangle Park, and Oak Ridge. At Oak Ridge, the focus has been on measuring deposition and exploring chemical transformation mechanisms, especially for high latitudes. Mercury oxidation investigation in Antarctica are now planned. These will begin with mercury speciation measurements at the coast (McMurdo) in October to investigate mercury oxidation by bromine. Mercury speciation measurements inland at the South Pole station from November to January will follow, investigating potential mercury oxidation by the hydroxyl radical (OH). brooks@atdd.noaa.gov

Mercury in the southeast is also being addressed at Oak Ridge. In June atmospheric mercury speciation equipment will be installed at Tuscaloosa AL. Ship-borne measurements off the Alabama coast will follow in July. These measurements will complement the summertime mercury concentrations at Oak Ridge and the Great Smoky Mountain National Park (measured in 2002). The ship-borne measurements will explore the rate of mercury oxidation in the remote marine boundary layer over the Gulf of Mexico. Seafood from this area of the Gulf is known to contain elevated mercury levels. <u>brooks@atdd.noaa.gov</u>, Lindberg, ORNL, Gabriel, Univ. of AL)

At Silver Spring, a modeling analysis of the transport and deposition of mercury to Lake Champlain was carried out. The work parallels similar assessments for the Great Lakes. Results were presented and discussed at a recent meeting/workshop in Burlington, VT dealing with science and policy issues regarding atmospheric deposition to Lake Champlain. The modeling results were evaluated by comparison against ambient monitoring data collected at Underhill Center, VT, near the lake. Very good agreement was observed between the modeled and measured data. A manuscript is being prepared. <u>mark.cohen@noaa.gov</u>

The Chesapeake Bay has also been addressed. Mark Cohen recently participated in and gave a presentation at the Workshop on Mercury and Methylmercury in Maryland's Environment, at the Maryland Department of Natural Resources in Annapolis, MD. An analysis of the transport and deposition of mercury to the Chesapeake Bay and other receptors in the mid-Atlantic region is being prepared. <u>mark.cohen@noaa.gov</u>

At Research Triangle Park, Eulerian modeling approaches are being developed, in the context of Models-3. In May, there was need to address aspects of the Clear Skies Act (CSA). On May 20, the Electric Power Research Institute (EPRI) presented to the EPA a report on their recent cost/benefit analysis of the proposed mercury emission control regulations under existing rules and under the proposed Clear Skies Act legislation forwarded by the White House (now a bill in Congress). EPRI described some rather controversial results. They estimated that CSA controls on the U.S. coal-fired electric power generation industry would reduce domestic mercury deposition by only 1.5%. A cursory analysis of modeling results in EPA's Mercury Study Report to Congress in 1997 suggests a figure of 15%, an order of magnitude higher. These EPA estimates were obtained using REMSAD, a commercial model developed by SAI, instead of the ASMD CMAQ-based mercury model. An analysis of differences between the CMAQ and REMSAD mercury model formulations and expected annual average results is being performed, in advance of a meeting (called by OMB) on June 6 to discuss the matter. <u>russell.bullock@noaa.gov</u>

4. Angell Symposium and SPARC Workshop Planned for November 4 and 5, 2003. Plans are underway for two international, one-day meetings to be held at NOAA in Silver Spring in November. The Jim Angell 80th Birthday Symposium will be held Tuesday November 4 to celebrate Jim's career and to recognize and review his scientific contributions in many areas of atmospheric research, particularly in observational studies of climate. For details see www.arl.noaa.gov/ss/climate/AngellSymposium.html. The following day, the WMO Stratospheric Processes and their Role in Climate (SPARC) Programme will hold a Workshop on Understanding Seasonal Temperature Trends in the Stratosphere. The workshop will focus on understanding stratospheric temperature trends and their causes and will also serve as a forum for organizing the future directions of the

SPARC Initiative on Stratospheric Indicators of Climate Change. More information is at <u>www.arl.noaa.gov/ss/climate/SPARCWorkshop.html</u>. The Air Resources Laboratory and WMO/SPARC are sponsoring the meetings. <u>dian.seidel@noaa.gov</u>

Silver Spring

5. *HYSPLIT – New Capabilities.* Although the option to initialize HYSPLIT with concentration data has been available for several years, the file was always created from a previous simulation. This file can now be created from measurement data. In conjunction with the original initialization option, the initialization file may contain multiple time periods, so that assimilation takes place when the model time matches the data in the file. Animation capabilities have been enhanced in the process.

A simple program was created to interpolate air concentration measurement data for use in HYSPLIT model initialization. Three options are available. The individual station may be directly converted to one mass point at each sampling location, the observations can be represented by multiple points randomly distributed, or the individual station data may be interpolated to a fixed grid. The output frequency corresponds to that of the input data unless a finer temporal resolution is specified. Future versions of the program could include meteorological information to assist in interpolation.

In response to increasing pressure for more qualitative and visual displays, three new programs (horizontal, vertical, and cross-section views) were developed to show pollutant distributions. Minor modifications were made to the HYSPLIT code to permit position information at multiple time periods to be output to the same file, again simplifying he preparation of animated presentations. <u>roland.draxler@noaa.gov</u>

6. Integrated HYSPLIT Package Submitted to NCEP. Programs have been submitted to NCEP to consolidate their operational dispersion capabilities and thereby unify the currently separate volcanic ash and radiological programs. A common framework should simplify operational support and upkeep at NCEP and further development at ARL. It will also facilitate application of new capabilities or output formats to the different simulations, e.g. volcanic ash or radioactivity. In the new system a single HYSPLIT program will be used for all dispersion simulations. For volcanic ash, this is a change in dispersion model from VAFTAD, though this may not be evident to the end-user since the output graphics are in the same format as the current VAFTAD output. For radiological applications (RSMC), in addition to a HYSPLIT upgrade, all output graphics will be in postscript format rather than NCAR graphics. Features of the integrated system include choice of input meteorological data, volcano database of latitudes and longitudes, and the ability to call up inputs from a recent previous run to make incremental changes for an update.

NCEP operationally creates global forecast data in the "ARL-format" for VAFTAD and HYSPLIT. These data are 6-hourly, 191 km, and on mandatory pressure levels. A new program has been submitted to generate higher resolution data. Once NCEP has implemented the new HYSPLIT package and VAFTAD is no longer being used, the current AVN forecast will not be needed. The new data are 3-hourly, on a one degree latitude-longitude grid, and with improved resolution in the vertical. <u>barbara.stunder@noaa.gov</u>

7. Volcanic Ash Dispersion Forecasts. The Washington Volcanic Ash Advisory Center (VAAC, NOAA NCEP/NESDIS) has issued many VAFTAD forecasts for the lengthy eruption of the volcano Anatahan in the Northern Mariana Islands. The volcano is about 400 km north of Guam. For the initial day or two of the eruption, the estimated top of the ash column was around 35,000 ft (~10.5 km), thereafter at most about 20,000 ft (~5.8 km). The eruption continues, but since the lower level eruption is generally not a significant issue for aviation, the VAAC is only issuing text advisories, with no graphical dispersion forecasts. barbara.stunder@noaa.gov

8. Potential Intensities of Tropical Cyclones: An analysis has been completed of the potential intensity of tropical cyclones, as calculated from thermodynamic principles using radiosonde data at 14 tropical island locations. The calculated potential intensity shows only small, statistically insignificant trends. Both reanalysis and radiosonde potential intensities show similar interannual variability in most regions, much of which appears to be related to ENSO and other changes in sea surface temperature. Comparison with results derived from NCEP reanalysis data suggests that the reanalysis-based results may sometimes overstate the potential intensity in at least some regions. <u>melissa.free@noaa.gov</u>

9. Norbert Gerbier-MUMM International Award for 2003. On May 26, 2003, the World Meteorological Organization's Executive Council, at its fifty-fourth session, conferred the Norbert Gerbier-MUMM International Award for 2003 on Dr. V. Ramaswamy (NOAA/GFDL) and co-authors (including Jim Angell and Dian Seidel), in a ceremony at WMO headquarters in Geneva, for the paper:

Ramaswamy, V., M.-L. Chanin, J. Angell, J. Barnett, D. Gaffen, M. Gelman, P. Kekhut, Y. Koshelkov, K. Labitzke, J.-J. R. Lin, A. O'Neill, J. Nash, W. Randel, R. Rood, K. Shine, M. Shiotani, and R. Swinbank, 2001: Stratospheric temperature trends: Observations and model simulations. Rev. Geophys., 39, 71-122.

10. Layer-mean Temperature on the Web. Work is nearly completed on refining the seasonal and annual temperature anomalies (in hundredths of a degree Celsius) obtained from a 63-station global radiosonde network for the period 1958-2003, as well as the temperature anomalies for the same period obtained from the 54-station network that results from exclusion of 9 anomalous tropical stations. In the case of the 63-station network, layer-mean temperature anomalies (obtained from the difference in geopotential height, or thickness, between constant pressure surfaces at individual radiosonde stations and application of the hydrostatic equation) are presented for five layers, two in the troposphere, two in he lower stratosphere, and one spanning the tropopause. The analysis is for 8 climate zones, hemispheres and globe. In the case of the 54-station network, the data presentation is more compact, with layer-mean temperature anomalies presented only for troposphere, tropopause, and low stratosphere layers, and for only polar, temperate and tropical climate zones, hemispheres and globe. Comparison with satellite and other radiosonde datasets suggests that the 54-station network provides more representative estimates of tropical, hemispheric and global temperature trend than the 63-station network, particularly in the tropopause layer but also in low stratosphere and troposphere. (Jim Angell, 301 713 0295, x127)

Boulder

11. SURFRAD/ISIS. The Bondville SURFRAD 2003 instrument exchange was completed on May 21. All equipment, support structures, and electronics for the new SURFRAD station at Sioux Falls, South Dakota, were assembled and readied for the installation. The new station will be installed on the grounds of the EROS Data Center Two vans filled with equipment will leave on June 3. The installation will take about eight days. The USGS, which operates EROS, is helping to cover the travel costs. (John Augustine, 303 497 6415)

Oak Ridge

12. *Terrestrial Carbon Program*. Data collection at the Walker Branch Site enjoyed outage-free service with full data recovery. Progress continues on the CHESS site's logistics. All but three poles have been installed to carry the power line. Placement of the remaining three, and arrival of power, awaits sufficiently dry soil low on the hill. The rebar cage for the tower base has been placed in the excavation, and the concrete forms have been positioned around it. The base and forms will be leveled, and the base's orientation will receive a final check before concrete is poured. <u>meyers@atdd.noaa.gov</u>

13. Canaan Valley. Deposition of nitrogen species to the surface in the Canaan Valley, WV was measured during the 2002 Intensive Field Study. Initial analysis aims to quantify the dry-deposition component, measured by relaxed eddy accumulation. Analysis of the wet-deposition measurements will follow. vogel@atdd.noaa.gov, Meyers

14. East Tennessee Ozone Study (ETOS). Preparation has begun to use the NOAA Twin Otter at Knoxville to fly approximately 16 hours in support of ETOS. This will follow the Joint Urban 2003 experiment in July. For ETOS we will be field-testing a new ozone instrument and comparing it with the two TECO instruments on board. gunter@atdd.noaa.gov, McMillen)

15. *HYSPLIT Atmospheric Dispersion Model.* A HYSPLIT dispersion system was built this month for Bill Petersen of NOAA/EPA/RTP. Several improvements were made to the existing system, including an improved concentration plotting routine. <u>dumas@atdd.noaa.gov</u>, Pendergrass, and Petersen/RTP

16. *Italian National Research Council Sky Arrow*. Work continues on the three MFP systems that are being built for Enzo Magliulo of ISAFoM-CNR (Italian National Research Council, Institute for Agricultural and Forest Meteorology). All necessary parts have been acquired and auxiliary boxes and probe assemblies are being manufactured. <u>auble@atdd.noaa.gov</u>, Brooks, Dumas, Ludwig, and Mayhew

17. NOAA Atmospheric Dispersion System (NADS). The survey of current emergency-response modeling practice for atmospheric transport and dispersion has been edited in response to reviewers' comments and will be sent for publication as a NOAA Technical Memorandum. The report will serve as a resource from which to draw and justify recommendations regarding the expansion of NOAA's Atmospheric Dispersion System to include optimal emergency-response forecasting on scales of 3 km to 30 km. <u>dobosy@atdd.noaa.gov</u>

18. U.S. Climate Reference Network. On May 13th, Michael Black, Mark Brewer, Keith Bryant and Blake Randolph left ATDD to install sites at Palestine, TX; Sandhills State Park, TX; and Socorro, NM. The site at Palestine will be solar powered and include a new battery enclosure which houses four 100 amp hour batteries instead of the standard AC-charged site, which houses two batteries. These sites were completed and transmitting data by May 25th. (Black, Brewer, Bryant, and Randolph)

Mark Hall attended a meeting in Boulder, CO to discuss issues associated with the Geonor precipitation gauge. Participants included users from Sweden, Canada, and the US. Representatives were also there from Campbell Scientific and Geonor. Betsy Weatherhead of NOAA is preparing a summary. <u>hall@atdd.noaa.gov</u>

One of the CRN technicians took another position at ATDD associated with the DCNet program. His nowvacant position will be advertised and filled in the next few months. Another technician is planning an extended vacation in Alaska this summer. In order to continue the site installations, two 5-month temporary technician positions are being filled. <u>hosker@atdd.noaa.gov</u>, Hall, Shifflett

Research Triangle Park

19. Community Multiscale Air Quality Model (CMAQ). Simulations were performed using a version of the Community Multiscale Air Quality (CMAQ) model capable of running on a new12-processor Linux Beowulf cluster. The model included the Carbon Bond IV (CB-IV) chemical mechanism, a 24-layer vertical structure and a U.S. continental domain with a 36-km grid cell resolution. During April and May 2003, simulations for January 1 through February 19, 2002, were completed and analyzed. Run times varied between 1.86 and 3.00 hours and averaged 2.20 hours for a 24-hour simulation. These simulations are being conducted as part of the aerosol nitrate research of CMAQ. (Michelle Mebust, 919 541 0833)

Improvements to the CMAQ plume dynamics model (PDM) are being made. Code revisions have been designed to allow for different plume release rates than the current hourly rate. Analyses have revealed that the wind direction shear provides a major contribution to the overall growth of plumes at large downwind distances during the day, while turbulence processes are more dominant closer to a point source. The next steps will be to perform test simulations with PDM data files containing different plume release rates. Ongoing analyses of the output concentrations of chemical and aerosol species are also being performed and additional applications are planned. (James Godowitch, 919 541 4802)

The Community Multiscale Air Quality (CMAQ) model for air toxics is being adapted to run on the IBM/SP2, the computing platform to be used for the National Air Toxics Assessment (NATA). Work will benchmark model performance and results against previous calculations on Linux-based workstations. It will also incorporate most of the changes in the pending 2003 summer release of CMAQ. Further adaptations attempt to optimize model performance based on the number and configuration of vertical layers. This work determines what model configuration will be used in NATA. (William Hutzell, 919 541 3425)

A long-term strategy for future development of the CMAQ aerosol components has been outlined. Development efforts in FY 2004 will focus primarily on improving model performance against ambient measurements of carbonaceous aerosols. Calculations of aerosol organic carbon using the current CMAQ release consistently exceed atmospheric measurements. In addition, recently developed parameterizations of fugitive dust and marine particle emissions will be integrated into the CMAQ system in FY 2004. Incorporation of gravitational settling and coarse mode coagulation are also planned. A sectional representation of the aerosol size distribution will be tested against the modal distribution, which is the default representation in CMAQ. An option for users to select either the sectional or modal aerosol representation is planned for release in FY 2005. Enhancements to the aerosol thermodynamic module are also planned for FY 2005. (Prakash Bhave, 919 541 2194)

An interim version of the Community Multiscale Air Quality (CMAQ) modeling system was released in May 2003 to the public through the Community Modeling and Analysis System (CMAS) Center. The major changes and new features of this release are:

- I. Scripts to build and run CMAQ for MPICH Linux clusters
- II. Incorporation of the I/O API Version 2.2
- III. Some additional enhancements and bug fixes.

Also, a "release" of an optimized version of CMAQ was made to the National Center for Environmental Prediction (NCEP) air quality forecast development group. This version is fast, taking about 16 minutes to run a 24 hour simulation on the NCEP high-performance computers. This benchmark was for a 166X142X22 (grid columsXrowsXlayers) domain using 32 processors for a CB-IV mechanism without aerosols. The timing is well within NCEP's operational window although more testing is required to benchmark the full "end-to-end" system, which includes the Eta meteorological model Product-Generator and the PREMAQ, CMAQ's meteorology and emissions preprocessor for the air quality forecast version. The PREMAQ (pre-processor to CMAQ) code, which was developed by ASMD to perform grid and variable transformations, was set up to generate meteorologically dependent emissions in addition to the meteorological fields. This update to the PREMAQ code is the final intended change prior to the summer test period for the air quality forecast system. The new version of PREMAQ was run successfully on NCEP's operational hardware. NCEP is currently testing PREMAQ as part of the end-to-end system in preparation for the semi-operational cycling that will start in June. (Tanya Otte, 919 541 7533: Jeff Young, 919 541 3929; George Pouliot, 919 541 5475)

On May 7, a summary was presented by the EPA Office of Research and Development modeling staff to the Office of Air Quality Planning and Standards modeling staff of all activities that have been conducted over the last six months to improve CMAQ's ability to simulated wintertime nitrate concentrations values. Major

updates were made to the model''s dry deposition algorithms and its treatment of nitrate chemistry. The overpredictions that were on the order of a factor of 3 to 5, have been reduced to within a factor of two. There yet remains a bias to overpredict the nitrate concentrations, but further improvements will have to await findings from ongoing and future research activities. On May 28, a summary on CMAQ model improvements was presented to the OAQPS Emissions, Monitoring and Analysis Division's director and staff assigned to the Director of OAQPS. Besides providing the overview of activities, new results were presented that demonstrated that the dry deposition improvements made for simulating wintertime nitrate concentration values has also improved CMAQ's performance during summertime. Preliminary results were also presented of improvements to be obtained in simulating semi-organic aerosols (SOA). During June, updates to CMAQ's treatment of semi-organic aerosol completed for public release by late August. (John Irwin, 919 541 5682)

20. Secondary Organic Aerosol (SOA). A series of tests was conducted with the revised, so-called reversible, secondary organic aerosol (SOA) partitioning algorithm (i.e., an algorithm that allows for both condensation and evaporation of semi-volatile organic compounds from aerosols). These model simulations also included emission adjustment factors to more accurately quantify the amount of semi-volatile gases produced from olefins and alkanes with high carbon numbers. Two tests were conducted using the SAPRC99 chemical mechanism, a week-long winter period and a week-long summer period. The results showed a significant drop in SOA formation in both cases as compared to results obtained with the older, irreversible algorithm (i.e., one that accounted for condensation only). Although preliminary testing of the new SOA algorithm has been completed, work is continuing in this area. First, the treatment of dry deposition of the semi-volatiles and SOA is being re-assessed. The possibility exists that too much SOA may be deposited when the new reversible algorithm is used with the standard dry deposition treatment. Alternate methods for using a more representative dry deposition velocity for the SOA particles and the semi-volatile gases are being evaluated. Second, work is beginning on developing a more generalized method of incorporating the reversible equilibrium algorithm and emission adjustment factors and linking them to the gas-phase chemistry. Current plans call for the results of this effort to be included in the August 2003 CMAQ release. Finally, OAQPS raised the question of whether it was necessary to include SOA production from olefins and alkanes. In response, some rough calculations were made to compare the potential SOA production from these two classes of compounds as compared to aromatics. These calculations suggest that alkanes and olefins could potentially account for 20%-30% of total anthropogenic SOA production, and, hence, probably should be included explicitly. The results have been forwarded to OAQPS for their review. At present, plans are to include SOA production from these two compound groups in the August 2003 CMAQ release. (Gerald Gipson, 919 541 4181)

21. Community Modeling and Analysis System Center. The Community Modeling and Analysis System (CMAS) now resides at the Carolina Environmental Program (CEP) of the University of North Carolina at Chapel Hill. As a component of the university community, CMAS''s ability to serve as a not-for-profit service center and collaborative agent has improved. CMAS has redesigned its web site (www.cmascenter.org) to expand capacity and clarify navigation. This web site provides model releases, documentation, and user support. During May, CMAS released a revised version of the CMAQ modeling system that includes several software bug fixes and uses a single Input/Output Applications Programming Interface library for the Models-3 system. This resolves confusion from a separate library used by the other components of the Models-3 system. Plans for the second annual CMAS users workshop are complete. A call for presentation titles and extended abstracts is expected shortly. Training on the use of CMAQ and the new version 1.5 of the Sparse Matrix Operator Kernel Emission (SMOKE) model system will be offered in conjunction with the workshop. The workshop is scheduled for October 27-29, 2003, at the Holiday Inn, Research Triangle Park, NC. (Bill Benjey, 919 541 0821)

22. *Euler Backward Iterative (EBI) Solver for CMAQ.* Testing of the new EBI gas-phase chemistry solver for the Carbon Bond IV (CB-IV) mechanism in the Community Multiscale Air Quality (CMAQ) model has been completed. The final test consisted of modeling the Atlanta, Georgia. area using a 2-km modeling grid for a period of five days (July 10 through July 14, 1999). The largest difference in 1-hour ozone concentration

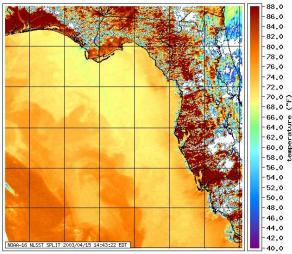
predicted with the EBI solver as compared to the slower Modified Euler Backward Iterative (MEBI) solver was about 1 ppb. The EBI solver reduced model run time by about 22% for this model configuration (no clouds or aerosols). Eliminating the transport of radicals in conjunction with the EBI solver reduced model run times by about 40% without any significant loss of accuracy. It must be emphasized, however, that these model speedups will be reduced if aerosols are included in the simulation. This final test completes work on the EBI solver for the CB-IV mechanism, and the new solver will be included with the next CMAQ public release scheduled for August 2003. (Gerald Gipson, 919 541 4181)

23. Testing New Planetary Boundary Layer (PBL) Scheme. The Asymmetric Convective Model (ACM) is a simple non-local closure PBL model which has been used in both meteorology and air quality grid models. However, when applied to air quality simulations the photochemistry in the PBL is significantly accelerated compared to using more traditional eddy diffusion models. This seems to be due to the rapid direct transport of ground-level emissions to all layers in the PBL. A new version is being tested that uses both non-local and local transport in convective conditions. This version should slow the PBL photochemistry while retaining some non-local transport. It is expected that this scheme will also retain the substantial computational speed advantage that ACM holds over eddy diffusion. (Jonathan Pleim, 919 541 1336)

24. Climate Impacts on Regional Air Quality (CIRAQ) Project. Progress has been made on several computer programs designed to manage a sizable (Tb) Regional Climate Model (MM5) data set that is expected to arrive over the next several months. The data management aspect of the program is necessary in order to streamline processing by the Meteorology-Chemistry Interface Processor (MCIP) for the Community Multiscale Air Quality (CMAQ) model. Additionally, a post-MCIP quality control and statistical module is partially complete. This module is being developed to provide assurance that the meteorological data is within some user controlled limit. Seasonal and regional statistics applied to air-quality related variables (user-controlled) will be another option encapsulated in the module, as well as visualization options of these analysis. During May, the initial version of the quality control code was successfully tested on a 1-month MCIP Data set. (Robert Gilliam, 919 541 4593)

25. *1-km Sea Temperature Ingestion for MM5 Simulations.* The initial version of a sea surface temperature processing utility for the Mesoscale Model Version 5 (MM5) model has been developed. The main reasoning behind this development is that typically MM5 uses coarse

(32 km or more) sea temperature data that is interpolated from larger scale models. In coastal areas, the sea temperature is one of the most dominating factors on the boundary-layer meteorology so it becomes critical to at least resolve it to the grid scale of the model. The first MM5 simulation in this study, planned to be completed in June 2003, is focused over Tampa Bay, Florida (April 20 - June It is expected that the more detailed sea 7, 2002). temperatures will improve the simulated coastal meteorology. The example image shows the 1-km sea temperature distribution off the west coast of Florida in April of 2002. A parallel simulation will be run without the high resolution temperature data. These will both be compared to observations and an assessment will be presented in a future paper. (Robert Gilliam, 919 541 4593)



26. *Emergency Response Modeling*. On April, 22 a drill was conducted to test procedures and practices within the EPA for responding to an emergency, as might occur if there were a terrorist incident. Following this, a meeting was held on April 24 to review needs for modeling. It was determined that communications during an emergency require at least two modelers present, one to handle the communications and one to perform

modeling activities. It was also determined that steps should be taken to automate as much possible the input and execution of the model for emergency response. To address this latter concern, EPA is implementing the modeling system, developed by the Atmospheric Turbulence and Diffusion Division of the NOAA Air Resources Laboratory. (John Irwin, 919 541 5682)

27. *Guideline on Air Quality Modeling.* On April 15, 2003, a Notice of Final Rulemaking was published by EPA that would update the *Guideline on Air Quality Modeling* to allow use of the CALPUFF modeling system for long-range transport (> 50 km) situations and on a case-by-case basis for complex wind situations. In the course of responding to this rulemaking activity, a series of discussions were held with EarthTech Inc. to insure that their web site was properly updated. EarthTech developed CALPUFF and distributes the modeling system freely to the public off their web site <u>http://www.src.com/calpuff/calpuff1.htm</u>. (John Irwin, 919 541 5682)

28. *Information Technology Research and Development.* Work continued on the development of the Multimedia Integration Modeling System (MIMS). MIMS provides software tools that support composing, applying, and evaluating complex systems of models, such as models of cross-media issues. A new version of the MIMS framework for configuring and executing models was posted to the project's web site. That version includes a wide variety of capabilities that were developed to support the multiple projects that are using the framework. In May, Steve initiated work to develop a prototype model evaluation toolkit. The intent of the toolkit is to provide specialized tools that could be used by multiple projects to evaluate model performance relative to observations. This prototype will be developed as new commands for the R statistical package allowing users to take advantage of R's existing capabilities for data manipulation, analysis, and plotting in conjunction with the new tools the MIMS project is developing. During the month, Steve also contributed to planning for EPA and Federal high performance computing capabilities. (Steven Fine, 919 541 0757)

A Fortran-based partial differential equation (PDE) solver subroutine provided by Multimedia Envirosoft Corp. was adapted to run as a stand-alone program on a Microsoft XP desktop system. Convergence tests were run for a sediment media example, and the response of solver convergence speed and solution to vertical resolution (number and thickness of sediment layers) were studied. When proper performance is achieved, the code will be passed to contractors at Argonne National Laboratory to compare against a JAVA implementation of the solver subroutine code. Full model definition and algorithm specification for a 4-compartment (media) hybrid (uniform and non-uniform) integrated multimedia pilot model was completed and passed to programmers at ANL for implementation. Delivery of a an initial implementation for AMD testing and evaluation is anticipated by July 1. (Ellen Cooter, 919 541 1334)

29. *Emissions Processing*. PREMAQ, a combined meteorological pre-processor and meteorologicallydependent emissions processing system, has been developed for the EPA/NOAA air quality forecasting project. Testing of the entire system including PREMAQ is underway at EPA and NOAA. Testing of the MIMS Spatial Allocator Program with the EPA released shape files has uncovered some issues on how the spatial allocator program processes the shape files. The Spatial Allocator program has been designed to provide users with a non-proprietary means of gridding spatial data for emission processing. Further testing and modifications to either the shape files or the allocator program will be needed so users can create their own surrogates for an arbitrary grid. Testing of the SMOKE version 1.5 is underway. Updates to the SMOKE code have been incorporated as they have become available and specification of inventories and input files for the 2001 National-Scale Air Toxics Assessment is underway. (George Pouliot, 919 541 5475)

William Benjey participated in planning the implementation of the dust emissions model being developed by Shan He and for a new model for estimation of ammonia emissions from fertilized fields. Geographic Information System-based input data required by both models is now being compiled and tested. The dust model will be applied to estimate particulate emissions from roads, construction, and agricultural fields using the new input data. Following testing the dust model will be installed as a module of the Sparse Matrix Operation Kernel Emission (SMOKE) model by the end of 2003. The model for ammonia emissions from fertilized fields will be developed and tested during the summer of 2003 following an intensive updated literature survey and recommendations exercise head by Tom Pierce. (Bill Benjey, 919 541 0821)

30. M3dry Subroutine. One issue identified while modifying the M3dry subroutine was the compatibility of the new dry deposition algorithm with MM5 runs not using the Pleim-Xu (PX) land-surface model. M3dry has now been updated to calculate stomatal resistance for non-PX cases. The PX model provides a canopy wetness parameter, which influences the resistances of soluble species. To compensate for the lack of this parameter in the non-PX runs, an approximation based on relative humidity and wind speed was added to M3dry to predict the presence of dew-wetted canopies. Rain or dew-wetted canopies are now assumed to remain wet throughout the night and to dry out after two hours during the day. (Donna Schwede, 919 541 3255; Jon Pleim, 919 541 1336)

31. *Global Change and Air Quality Research*. Research regarding regional meteorological analysis approaches for application to the MM5 meteorological model run in regional climate mode (MM5/RCM) output was begun. This will be the primary topic of the first regional climate scenario workgroup meeting, to be held in early June. Univariate as well as multivariate approaches are being considered and a preliminary set of MM5/RCM variables will be identified for extraction from the full output file. Atmospheric Sciences Modeling Division analyses will be coordinated with those of Pacific Northwest National Laboratory (PNNL). A meeting was held with Chris Geron of the EPA National Risk Management Research Laboratory Air Pollution Prevention and Control Division to discuss landuse/landcover change scenario research plans for global change applications. These plans were communicated to the EPA Global Change and Air Quality emissions workgroup. (Ellen Cooter, 919 541 1334)

The EPA Global Climate Change Program's air quality effects workgroup continued gathering information to guide projections of future year emissions. This activity is focusing on ways to minimize differences between projected emissions data resulting from different projection methodologies. (Bill Benjey, 919 541 0821)

32. Urban Dispersion Modeling. Computational fluid dynamics (CFD) simulations have been used to address the 9-11 collapse of the World Trade Center. These methods are relatively new to applications in environmental science because of the temporal and spatial scales, and the complex chaotic nature of the physical processes in environmental problems. CFD techniques can be employed to describe the flow of pollutants in the complex urban building environment. The simulations have the ability of closely matching the true geometry of the buildings and the "real world" physical processes. These simulations can be used directly or as a foundation for developing reliable simplified models for rapid risk assessment. The effort includes using actual field measurement data from New York, together with measurements from a scale-model of the WTC site in the Fluid Modeling Facility. (Alan Huber, 919 541 1338)

Idaho Falls

33. *Joint Urban-2003.* Preparations are in full swing for deployment to Oklahoma City next month. Sixty-five new samplers are being constructed along with 325 new cartridges into which they will be inserted when deployed. All new sample bags were purchased for the new samplers and for replacement of all bags in the existing cartridges, of which there are 667. The Tracer Analysis Facility (TAF) also underwent several tuning steps. The dynamic range was tested to see if it could be extended without a compromising residual contamination effect. Several sample loop sizes were also tested. Currently, the highest concentration that can be routinely measured is 35,000 ppt. Concentrations up to 200,000 ppt will require different handling.

Extensive testing was also undertaken to improve the method limit of detection (MLOD). The MLOD is the limit of detection applied to the entire handling and analysis method, from the initial cleaning of the bags, to their deployment in samplers and finally to their analysis on a gas chromatograph. Through additional cleaning

of the bags and other precautions, we were able to cut our MLOD at least in half. It is now comfortably at the SF_6 background level, which is 3 ppt.

The SF₆ tracer release mechanisms were prepared during May. Two puff release mechanisms were obtained from Dugway Proving Ground and inspected for adequate operation. Unfortunately, the two systems leaked a substantial amount of SF₆ and they also made a very loud bang when opened. The noise level was so high that there would be cause for alarm if these were used in downtown Oklahoma City. A balloon filling and bursting procedure was subsequently devised which would provide the same functionality without the noise. The continuous release mechanism was also prepared and tested.

The final draft of the experimental plan was received from the science team lead. The plan is rather complicated, the result of many divergent opinions of the modelers and the requirements of experimentalists. It will require high attention to detail when fielding our 150 bag samplers. We will also deploy 10 real-time SF_6 analyzers for measuring both puffs and plumes of SF_6 , as well as a sodar system. <u>kirk.clawson@noaa.gov</u> and staff)

34. CBLAST-High. Preparations continue for the upcoming 2003 hurricane season. Lab work on the BAT instruments and data system for the P3 was completed. Calibrations were completed. A battery of tests to assure the equipment is working properly has been conducted. The equipment was shipped to NOAA's Aircraft Operations Center, MacDill AFB at the end of May. Installation is scheduled for the first of June with test flights scheduled for late July. Changes/modifications to the system that was flown during the 2002 hurricane season include an improved aluminum hemisphere that is more robust and less labor intensive (and therefore less expensive) in construction, improved mirrors for the IRGA (the original silver-plated mirrors were badly corroded), and an improved software package for the data system. Upgrades continue on the data system software; these are expected to be completed prior to the test flight in July. jeff.french@noaa.gov

35. *ET Probe.* Further field tests of the ET probe were conducted in May. The tests performed in late April showed some minor problems with the data acquisition system. These were quickly fixed. A more serious problem cropped up early in May when additional road tests were performed with the ET probe mounted on a pickup truck. The system worked well for the first few minutes on the road, but then started to show unusual voltage fluctuations which corrupted the pressure data. Annoyingly, the system often started working properly again after the truck was driven back to FRD and parked. Eventually, it was found that the USB hub used for communication between the AD boards and the notebook computer was overheating. This hub must be "self-powered", because the computer cannot supply sufficient power through its USB port to run both AD boards. Power was supplied by a DC/AC inverter connected to the truck's battery, and this supply suffered from large voltage surges depending on engine output. The problem was fixed by running the entire ET probe system off a small gasoline generator placed in the truck's bed. A highly successful field test was conducted on 15 May, when the truck-mounted ET probe was driven out to INEEL and operated at a fixed location for several hours near a sonic anemometer. Ambient winds were about 10-20 m/s on this day, which is sufficient for the probe to operate properly. richard.eckman@noaa.gov, Tom Strong

Las Vegas

36. *Mesoscale Modeling*. NV-RAMS ran to completion on the University of Nevada-Las Vegas computer system 27 of 31 days (an 87% completion factor). The incomplete days were due to unavailable ETA initialization datasets from NCEP; they installed new computers and all the bugs were not worked out. Data are continuing to be saved daily, and backed up to CD monthly. The 12z model run has been working well. Near the end of the month the run began taking twice as long to run. The problem is being investigated; it may be due to increased computer usage. All graphics for the 2km and 8km grids have been put into production test bed. (Walt Schalk, 702 295 1262)