NOAA Air Resources Laboratory
Monthly Activity Report

July 2007

Contents

1. Highlight -- Measurement of the Net Exchange and In-Canopy Source/Link Characteristics of Ammonia Fluxes in an Agricultural Setting. Scientists from the Atmospheric Sciences Modeling Division (ASMD), the Atmospheric Turbulence and Diffusion Division (ATDD), ARL Headquarters; the U.S. Environmental Protection Agency National Risk Management Research Laboratory; and collaborators from other organizations (with support from the U.S. Department of Agriculture) completed a field measurement campaign. The campaign, conducted at a 500-acre corn field in Lillington, North Carolina, investigated ammonia flux sources, sinks and regulation in a commercial agricultural setting. High-quality in- and above-canopy turbulence profiles, leaf temperature profiles, the in-canopy ammonia concentration gradient, and multiple measures of the atmospheric-canopy ammonia flux were collected throughout the growing season. Leaf and soil chemistry measurements were taken to better understand ammonia deposition over a wet canopy and

the compensation point in the ammonia flux over a corn canopy. Instrumentation included a gradient system utilizing annular denuders to collect ammonia, nitric acid, and sulfur dioxide along with filter packs to collect particulate nitrate and sulfate ($D_p < 2.5$ μm). Two-hour samples were collected four times each day to capture concentrations representative of morning, mid-morning, afternoon and late afternoon conditions and were shipped to the ATDD chemistry laboratory for ion chromatography analysis. Supplementary micrometeorological and fast-response ozone measurements were also collected. Two intensive studies were conducted from May 24 through June 4 (pre- and post- fertilization) and July 9 through July 15 (full canopy conditions). These data, in conjunction with detailed canopy turbulence and scalar exchange models, will be used to estimate the relative influence of canopy and soil sources/sinks on the overall atmospheric-canopy ammonia flux under a wide range of meteorological and ambient ammonia concentration conditions. The findings of this study will also be used to evaluate and improve algorithms to predict the bi-directional exchange of ammonia from agricultural land cover types in the Community Multi-scale Air Quality model (CMAQ). jesse.bash@noaa.gov; donna.schwede@noaa.gov; tilden.meyers@noaa.gov; latoya.myles@noaa.gov; laureen.gunter@noaa.gov

2. Highlight -- National Ambient Air Quality Standards. Marc Pitchford participated in a kick-off workshop for the review of the particulate matter PM Secondary National Ambient Air Quality Standards (NAAQS) on July 16, and a peer review workshop for the Integrated Science Assessment for the sulfur dioxide and nitrogen oxides (SO_2 and NO_x) Secondary NAAQS from July 17 to 19 in Chapel Hill, NC. For the PM workshop, Dr. Pitchford summarized the relationship between PM and visibility impacts, then lead a discussion among the other experts of the technical information that should be included in an Integrated Science Assessment in order to determine whether a Secondary NAAQS that would protect visibility in urban areas is supportable. For the SO_x - NO_x workshop, Dr. Pitchford summarized the Draft Visibility Impacts chapter that he'd authored for Integrated Science Assessment. Among the recent findings discussed are the surprisingly high concentrations of particulate ammonium nitrate in a multi-state region of Midwest centered on Iowa. There is evidence that high ammonia emissions density associated with animal agriculture combined with the low winter temperature in that region are responsible for the high levels of ammonium nitrate. marc.pitchford@noaa.gov

Air Resources Laboratory Headquarters, Silver Spring

3. CHEMTAP Update. NOS HAZMAT presented some preliminary results of their chemical accident planning tool using HYSPLIT as the dispersion modeling component at the recent GMU conference. A DVD with more detailed results was given to us and a detailed review of their computational approach resulted in several suggestions regarding concentration layers and particle release rates that should be used to optimize their calculations. roland.draxler@noaa.gov

4. LAPS Update. Based upon an initial review of the 1.5 km LAPS calculations by GSD for the 4Washington D.C. metropolitan area, we suggested that they increase the number of data levels output in the boundary layer. Further, the dispersion calculations using those data seemed to show certain biases (slow transport, little mixing). However, after discussion with GSD we realized that we were using the raw LAPS data rather than the balanced output fields. Using the balanced fields resolved many of these issues. roland.draxler@noaa.gov

5. HYSPLIT Update. In anticipation of several upcoming HYSPLIT workshops, two new post-processing modules for source-attribution computations were added as options to the graphical user interface. In the first approach, HYSPLIT is run multiple times in a backward integration for periods that correspond with individual measured sampling data. The results are then averaged to determine the most likely source region. In the second approach, the source-receptor coefficient matrix is solved for the source term vector given a measured data vector where the matrix values are the dilution factors computed by HYSPLIT for each source-receptor pair. roland.draxler@noaa.gov

6. Review Article on Tropical Widening. A "progress article" reviewing the recent literature, from both modeling and observational studies, on the widening of the tropical belt as an aspect of global climate change has been submitted to the new journal Nature Geoscience. Co-authors include Qiang Fu (U. Washington), Bill Randel (NCAR) and Thomas Reichler (U. Utah). dian.seidel@noaa.gov

Atmospheric Turbulence & Diffusion Division (ATDD), Oak Ridge

7. Climate. The Climate Reference Network expanded by four sites in four states: Missouri, Minnesota, South Dakota, and Wyoming. The total is now about 110 distributed over all 50 states. Meanwhile the busy annual maintenance schedule continued, enforcing the strict quality control. There were 26 sites visited in the western and northern states, best handled in summer. mark.e.hall@noaa.gov

The ongoing Oak Forest Classic Summer Experiment in Oklahoma studies the contributions of large vegetation regimes to strong convective storms through air-surface exchange. Such storms are an important climate feature of the southern plains of North America. ATDD installed and is operating instruments to monitor the budgets of water, heat, and carbon in an oak-forest reservation near Okmulgee, in eastern Oklahoma. tim.wilson@noaa.gov

8. Air Quality. Agricultural ammonia may be a nutrient or a nuisance, or both if it escapes to the atmosphere from the field where it is needed and gets deposited into lakes and streams. Ammonia emission from a fertilized mature 200 ha stand of maize was measured in July in North Carolina, along with nitrates and sulfates with which ammonia readily combines. This intensive experiment included sampling of soil and leaf chemistry by collaborators from EPA and USDA. The work seeks to enhance farmers' efficient use of a costly resource and to improve air quality over the extensive parts of North America devoted to agriculture. laureen.gunter@noaa.gov

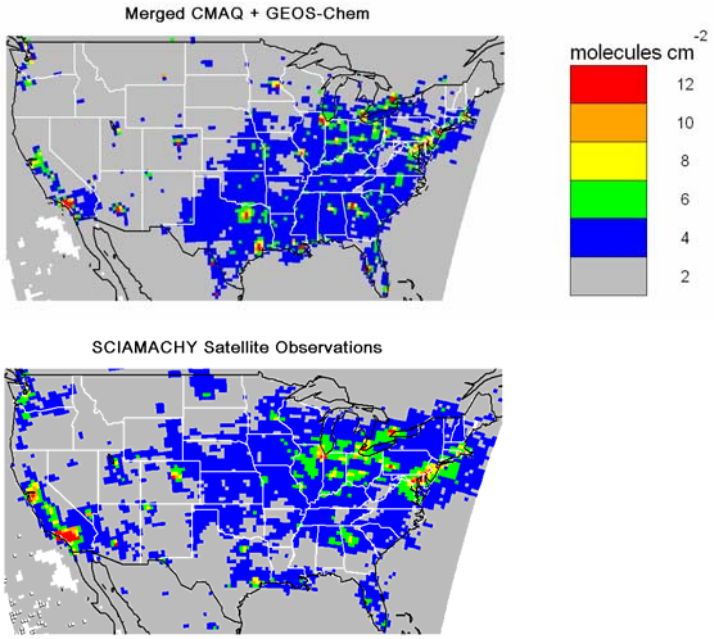
Atmospheric mercury's chemistry is strongly linked to halogen (specifically bromine) chemistry even at summit Greenland (3125 m MSL, 600 km from the ocean). Reactive gaseous mercury was strongly correlated to BrO, which peaked diurnally at peak incoming solar radiation. Fine-particulate mercury (24-hour) was correlated to aerosol bromine, which was anti-correlated with air temperature. steve.brooks@noaa.gov

Atmospheric Sciences Modeling Division (ASMD), Research Triangle Park

9. Regional-Global Model NO_2 Column Density for Comparison with Satellite Observations and Inverse Modeling of NO_x Emissions. With the help of collaborators from Dalhousie University and Harvard University, division scientists have developed a merged regional-global model NO_2 column

density for comparison with satellite observations. The global model (GEOS-Chem) contains a more detailed representation of the upper troposphere emissions and the exchange processes between the stratosphere and the troposphere. The more fine-grained horizontal resolution of the regional model (CMAQ) better captures the urban and rural gradients. The merged fields are highly correlated (0.78) with the satellite observations from SCIAMACHY over the eastern United States during the summer of 2004. This merged dataset can help users of the satellite data more readily separate the impacts of surface NO_2 emissions and aloft biogenic sources.

Using these results, inverse calculations have been performed to estimate what NO_x emission changes would be needed to bring the modeled NO_2 columns and satellite data into better agreement. Three independent versions of the modeled NO_2 columns were tested for the inverse calculations: comparing SCIAMACHY results directly with CMAQ predictions; enhancing CMAQ predictions with ICARTT observations for the upper troposphere; and enhancing CMAQ predictions with GEOS-CHEM results for the upper troposphere. The results are significantly different for the three cases. Comparison to data collected by the SEARCH monitoring network during this period does not single out which results are more accurate, but instead highlights the level of uncertainty inherent in modeling the tropospheric column budget of NO_2. A draft of a manuscript summarizing this work is being prepared. rob.pinder@noaa.gov, sergey.napelenok@noaa.gov



10. Air Quality Forecast Model Development, Testing, and Analysis. Analysis of daily surface level O_3 forecast from experimental NAM-CMAQ forecast over the Continental United Sates was continued. Two modifications were introduced in the PREMAQ to correct errors: (1) a mesophyll resistance term was added in the calculation of the deposition velocities for NO, NO_2, and CO, and (2) modifications were introduced in the plume-rise calculation to use the correct pressure field on the hybrid coordinate. The latter change had minimal impact on the representation of plume rise of point source emissions and subsequent predicted O_3. However, the changes in the deposition

velocity calculations for NO and NO_2 resulted in widespread regional impacts on predicted O_3 with a general enhancement of 2-3 ppb for the daily maximum 8-hour O_3. The modification also resulted in enhancements in predicted ambient CO concentrations due to reduced deposition velocity. Operational readiness briefings on the Continental U.S. experimental forecast systems are planned for later this summer by the National Weather Service. jonathon.pleim@noaa.gov, rohit.mathur@noaa.gov, george.pouliot@noaa.gov

11. Bi-directional Mercury Exchange in the Community Multiscale Air Quality (CMAQ) Model Over Surface Waters. Natural emissions of gaseous elemental mercury (GEM) are estimated to be as large as or larger than the total anthropogenic mercury emissions to the atmosphere. Measurements of dissolved gaseous elemental mercury concentrations in surface waters are higher than predicted by Henry's constant. Air quality models currently parameterize the atmosphere-surface water exchange of mercury by eliminating the atmospheric deposition and characterizing the evasion process as a function of meteorological parameters and/or constant surface water dissolved GEM concentration. Recent flux chamber measurements indicate a seasonal pattern in the atmospheric – surface water exchange of mercury, correlating with incoming solar radiation during the summer and with wind intensity during the winter. A mass conservative and physically descriptive multimedia bidirectional mercury exchange model is being developed for CMAQ to capture these processes. The wind driven atmosphere – surface water mercury fluxes are being parameterized using a two-film turbulent diffusion model, and a surface water photo-reduction scheme is being developed to better capture the enrichment of surface water with dissolved GEM. Both of these processes require mercury concentrations in the surface waters and a dynamic surface media layer to simulate surface accumulation and depletion of mercury from deposition and evasion. These processes have been added to CMAQ. jesse.bash@noaa.gov

12. Community Modeling and Analysis System (CMAS) 2007 Annual Conference. The agenda has been announced for the 6th Annual CMAS User's Conference scheduled for October 1-3, 2007, at the Friday Center in Chapel Hill, NC. Papers from all facets of air quality modeling were submitted, including both platform and poster presentations. The focus for this year's conference is a special session on "advances in understanding the sensitivity of air quality models to meteorological inputs." It is expected that at least 20 papers addressing this topic will be developed into full articles for consideration of their publication in a special issue of Environmental Fluid Mechanics Journal. S.T. Rao will be the Guest Editor of this special issue. Other sessions include air quality model developments, emission inventory modeling and analyses, air quality forecasting, model evaluation and analysis, climate variability and air quality, integrated modeling systems for environmental decision support, and urban database development and air quality applications. CMAS will offer training in the use of the Community Multiscale Air Quality (CMAQ) model and the Sparse Matrix Operator Kernel Emission (SMOKE) model in conjunction with the conference. As of the beginning of August, 132 paper titles and abstracts had been submitted, and 145 participants had registered from 11 countries. Registration for attendance will remain open through the conference, although reduced registration rates continues only through September 4, 2007. Registration details, logistics, and other details are available on the Internet at http://www.cmascenter.org. william.benjey@noaa.gov, st.rao@noaa.gov

13. Development of Suitable Method for Measurement of Dry Deposition of Elemental and Reactive Gaseous Mercury to Coastal Ecosystems. A collaborative measurement campaign

between NOAA/ASMD and the University of Connecticut's Department of Marine Science has been initiated. The objective of this two-year study is to develop and to evaluate suitable micro-meteorological flux techniques to measure elemental and reactive gaseous mercury and to provide high-quality speciated mercury flux measurements in the marine boundary layer. Relaxed eddy accumulation and modified Bowen ratio measurements of the elemental mercury, reactive gaseous mercury, CO_2 , and H_2O fluxes will be taken at Avery Point, Connecticut during summer, 2008 and at the Narragansett Bay National Estuarine Research Reserve during summer, 2009 The results of this measurement campaign, funded by the NOAA Cooperative Institute for Coastal and Estuarine Environmental Technology (CICEET), will provide the first micrometeorological measurements of speciated and elemental mercury loading to sensitive estuary systems. These measurements will support further development and evaluation of the bi-directional atmosphere-oceanic mercury exchange model for the Community Multiscale Air Quality (CMAQ). jesse.bash@noaa.gov

Field Research Division (FRD), Idaho Falls

14. Urban Dispersion Program. The manuscript "Atmospheric Flow Decoupling and its Effects on Urban Plume Dispersion" is still under review at the journal Boundary Layer Meteorology. The manuscript "Plume Dispersion Anomalies in a Nocturnal Urban Boundary Layer in Complex Terrain" is still undergoing ARL review. A draft manuscript "Probability Density Functions and Peak-to-Mean Ratios for Tracer Plumes in an Urban Boundary Layer" has been completed and is presently undergoing internal FRD review. This manuscript contains some material leftover from the first paper listed above and incorporates some new material from Joint Urban 2003. One key finding was that peak-to-mean values, while usually less than five, were commonly as high as 5-10 and ranged upward as high as 58.3. It was also found that probability distributions ranged from strongly positively skewed near the margins of the plume or close to the source to only weakly skewed in the more well-mixed portions of the plume at greater distances from the source during the nighttime. These results have implications for assessing the hazards posed by toxic airborne releases and offer guidance for the development of urban dispersion models. dennis.finn@noaa.gov

15. Perfluorocarbon Tracer Analysis Development. The 250, 4000, and 100,000 pptv sample stability tests continued. These tests have been in progress for 6 months now and the data still indicate that sample deterioration is minimal. We are still trying to resolve some chromatogram interference issues for PDCB at lower pptv levels. dennis.finn@noaa.gov and Roger Carter

16. Emergency Operations Center (EOC). A large wildfire broke out on the East Butte of the INL the evening of 18 July. The EOC was activated shortly after it was first discovered and remained operational for 26 hours. The blaze was brought under control on the evening of 19 July after burning 9,436 acres. The cause of the blaze is still being investigated. FRD provided timely short range forecasts to EOC personnel during the activation. jason.rich@noaa.gov, Brad Reese, Rick Eckman, and Neil Hukari

17. ANSI /ANS-3.11-2005 Deficiencies. The criteria for gathering and assembling meteorological information at the Department of Energy nuclear facilities are contained in the document ANSI/ANS-3.11-2005. It was found during the 2004 Assist Team Visit from the DOE Meteorological Council that 22 out of the 23 objectives in the ANSI-ANS-3.11 guide were being met. The only objective not being met involved using the root mean square methodology in

determining the total system accuracy. This deficiency is now being addressed. A document describing all of the end to end errors and the associated root-mean-square error for each instrument in the meteorological data gathering system is being developed. In conjunction with this effort, modifications necessary to bring the existing "Semiannual Calibration and Maintenance Form" into compliance with ANSI/ANS-3.11 requirements are being implemented. randy.johnson@noaa.gov

18. Transport and Dispersion Modeling. FRD has continued its discussions with other ARL divisions and the CAMEO/ALOHA group within the National Ocean Service on improving HYSPLIT for local dispersion applications. Since both FRD and SORD have large mesonets, one of the main required improvements is a method of deriving a local 3D wind field that takes full advantage of these mesonets. One possibility is to use the NOAA Local Analysis and Prediction System (LAPS) to blend local observations with a 3D background wind field derived from a numerical forecast model. A copy of LAPS was obtained at FRD, but it was quickly determined that it is difficult to use. The main problem appears to be that LAPS is tightly integrated with other applications running at ESRL; other users have to duplicate the functionality of these other applications, which can be highly time consuming. Focus has now shifted to the WRF-Var system that is available as part of the overall WRF development effort. WRF-Var is a variational data assimilation system that can handle many of the same data inputs as LAPS. It has the advantage of being directly compatible with the existing WRF configuration at FRD. In addition, the NOAA Meteorological Assimilation Data Ingest System (MADIS) appears to provide utilities that convert observations from its database into a format compatible with WRF-Var. richard.eckman@noaa.gov

The 2006 annual dispersion estimates for the INL were completed in the first week of July. These model estimates are used to estimate possible exposures to individuals living in the area surrounding INL, and the results go into the annual site environmental report. richard.eckman@noaa.gov

Special Operations and Research Division (SORD), Las Vegas

19. Hollings Scholarship Intern. Jackson Switzer, a Hollings Scholarship Intern from the University of Alabama, completed his final research project under the supervision of W. Schalk. His report was entitled "Local-scale Comparison of ALOHA and HYSPLIT Dispersion Models Using WRF Windfields." In addition to the written report, Mr. Switzer also gave a PowerPoint presentation at the Hollings Scholarship meeting in Washington, D.C. on July 30. walter.w.schalk@noaa.gov

20. WRF Model. Version 1 of *ARWpost* was downloaded and installed. An error in the module v5d_module.f90 which caused the times in vis5d files to be 1 hour off was fixed. Worked progressed towards the use of vis5d and Unidata's Integrated Data Viewer (IDV) to visualize fields.

The [CO_2] in the WRF code was updated from a value representative of the early 1990's to 375 ppmv.

WRF 6-hour forecasts starting from 06 and 18 UTC were added to *meso* to prepare for running the model in cycling mode. kip.smith@noaa.gov

ARL is considering how to best keep its stakeholders informed about its activities. You could help the Lab share information with you more effectively, by sending a brief note to betty.wells@noaa.gov indicating if you find information in the monthly activity reports useful and if you have any suggestions for how we could more effectively provide the information that you need.