[1]Aeronomy Laboratory, National Oceanic and Atmospheric Administration, 325 Broadway, Boulder, CO 80305, United States

[2]Cooperative Institute for Research in the Environmental Sciences, The University of Colorado, Boulder, CO 80309, United States

This laboratory study focuses on new particle formation resulting from the oxidation of α-pinene. Using a Teflon reaction chamber (70 L), ultrafine (>3 nm dia.) particle formation was studied for α-pinene concentrations between $1x10^{-10}$ atm and $2.4x10^{-8}$ atm at ozone concentrations between $1.2x10^{-7}$ atm and $1.4x10^{-6}$ atm. Experimental timescales of 40 minutes allowed appropriate time to investigate particle formation and subsequent growth of nanometer size particles. New information is presented regarding: 1) the effect of oxidizing agent (O_3 or OH) on aerosol mass yield and new particle concentration; 2) measurements performed near atmospherically relevant concentrations; and 3) the dependence of water vapor on the α-pinene gas-phase oxidation mechanism and hygroscopic growth of new particles.

A41G-04 1115h INVITED

Secondary Organic Aerosol Formation: New Insights

Richard M Kamens (919-966-5452; kamens@unc.edu); Myoseon Jang (919-966-3861; mjang@email.unc.edu); Sangdon Lee (919-966-3861; goodlsd@email.unc.edu); Nadine Czoschke (919-966-3861; nadine@email.unc.edu); Sirakarn Leungsakul (919-966-3861; sleungsa@email.unc.edu); Di Hu (919-966-3861; dhu@email.unc.edu)

A discussion of some of the important issues related to secondary organic aerosol (SOA) formation is presented, and SOA formation is placed in a context of global fine aerosol sources. Outdoor smog chamber experiments are described for the purposes of exploring the effects of different types of background aerosols on SOA formation from the reaction of α-pinene with NO_x in the presence of natural sunlight. Experiments were carried out by first adding 20 to 200 $\mu g/m^3$ of background aerosols (such as diesel soot, wood smog, and ammonium sulfate seed particles) into $190m^3$, $140m^3$, and $25m^3$ Teflon film outdoor chambers prior to the addition of α-pinene and NO_x. SOA formation was monitored using a scanning mobility particle sizer (TSI-SMPS). Gas and particle phase products were sampled over the course of experiments using denuders and filters. Chamber results indicated that condensed SOA can dramatically alter the chemical composition of primary diesel soot particles as they age in the atmosphere. Since particle phase aldehyde chemistry has recently been implicated as a potentially large source of SOA (Jang and Kamens, et al., *Science* 2002), aerosol growth by the heterogeneous reactions of different organic carbonyls in the presence/absence of acidified seed aerosols was studied in a flow reactor and 500-liter Teflon bag system under dark conditions. The results from unsaturated carbonyl and dicarbonyl experiments indicate large increases in SOA formation in the presence of acidified aerosols. This has implications for both biogenic and aromatic systems that generate SOA.

A41G-05 1135h

Aldol Condensation of Volatile Carbonyl Compounds in Acidic Aerosols

Barbara Noziere[1] (305 361 4714; bnoziere@rsmas.miami.edu)

William Esteve[1] (305 361 4125; westeve@rsmas.miami.edu)

[1]Rosenstiel School for Marine and Atmospheric Science, Marine and Atmospheric Chemistry Division University of Miami, 4600 Rickenbacker Causeway, Miami, FL 33149, United States

Reactions of volatile organic compounds in acidic aerosols have been shown recently to be potentially important for organic aerosol formation and growth. Aldol condensation, the acid-catalyzed polymerization of carbonyl compounds, is a likely candidate to enhance the flux of organic matter from the gas phase to the condensed phase in the atmosphere. Until now these reactions have only been characterized for conditions relevant to synthesis (high acidities and liquid phase systems) and remote from atmospheric ones. In this work, the uptake of gas-phase acetone and 2,4pentanedione by sulfuric acid solutions has been measured at room temperature using a Rotated Wetted Wall Reactor coupled to a Mass Spectrometer. The aldol condensation rate constants for 2,4pentanedione measured so far for sulfuric acid solutions between 96 and 70 % wt. display a variation with acidity in agreement with what predicted in the organic chemical literature. The values of these constants, however, are much lower than expected for this compound, and comparable to the ones of acetone. Experiments are underway to complete this study to lower acidities and understand the discrepancies with the predicted reactivity.

A41G-06 1150h

Dissolution and Speciation of Oxygenated Organic Compounds in Sulfate Particles: Acetaldehyde

Rebecca R. Michelsen[1] (650-604-2793; rmichelsen@mail.arc.nasa.gov)

Samantha F.M. Ashbourn[1]

Laura T. Iraci[1]

[1]Earth Science Division NASA Ames Research Center, MS 245-5, Moffett Field, CA 94035-1000, United States

The uptake of small organic compounds by sulfate particles is enhanced by the speciation of the compounds in acidic aqueous solution. Acetaldehyde [CH_3CHO] exists in such solutions in several forms: molecular, hydrated, enolized, and protonated acetaldehyde. The contribution of these various dissolution pathways to the heterogeneous interactions of acetaldehyde with upper tropospheric sulfate solutions will be evaluated. The uptake of acetaldehyde by aqueous sulfuric acid has been studied via Knudsen cell experiments over ranges of temperature (210-250 K) and acid composition (40-80 wt. %) representative of the upper troposphere. The Henry's law solubility coefficients for acetaldehyde calculated from these data range from 10^2 to 10^5 M atm^{-1}. Results from the interaction of acetaldehyde with solutions of formaldehyde in sulfuric acid will be presented as well. The physical and chemical processes that affect organic uptake by aqueous aerosols will be explored, with the aim of evaluating organic species not yet studied in low temperature aqueous sulfuric acid.

A41G-07 1205h

Acid-catalyzed Heterogeneous Reactions in SOA Formation

Nga Lee Ng[1] (626 395 4476; ng@caltech.edu); Melita Keywood[1] (626 395 4476; meltia@cheme.caltech.edu); Varuntida Varutbangkul[1] (626 395 4476; tomotor@caltech.edu); Song Gao[1] (626 395 4476; sgao@caltech.edu); EthelMae Loewer[1] (626 395 4476; ethelmae@caltech.edu); Jason Surratt[1] (626 395 4476; surratt@caltech.edu); Flagan C Richard[1] (626 395 4383; flagan@cheme.caltech.edu); Seinfeld H John[1] (626 395 4635; seinfeld@caltech.edu)

[1]California Institute of Technology, 2100 E California Blvd, Pasadena, CA 91106, United States

The importance of heterogeneous reactions in secondary organic aerosol (SOA) formation has recently excited a great deal of interest in the aerosol community. Jang and Kamens (2001) showed enhanced aerosol yield from aldehydes, which can be produced by atmospheric photochemical reactions, in the presence of acidic seed. They suggest that the carbonyl functional groups of the aldehydes further react in the aerosol phase via hydration, polymerization, and hemiacetal/acetal formation with alcohols at an accelerated rate in the presence of acid. Jang et al. (2003) demonstrated similar results using a flow reactor and Czoschke et al. (in press) qualitatively showed increased yields for isoprene and alpha-pinene ozonolysis in the presence of acidic seed. While these findings are intriguing and important, the conditions under which the experiments were carried out were atmospherically unrealistic. A series of SOA formation experiments have been carried out in the Caltech Indoor Chamber Facility, which is comprised of dual 28 m^3 FEP Teflon chambers, with the flexibility to carry out both dark ozonolysis and photochemical OH oxidation reactions. Cycloheptene and alpha-pinene were oxidized in the presence of neutral seed under dry (<10% RH) and humid (50% RH) conditions and in the presence of acidic seed under humid (50% RH) conditions. The SOA yields for these experiments will be presented, and the extent of the influence of acid-catalyzed reactions on SOA yield will be discussed. Reference List 1. Cocker, D. R. III. and R. C. Flagan and J. H. Seinfeld, State-of-the-art chamber facility for studying atmospheric aerosol chemistry, Environmental Science and Technology, 35, 2594-2601, 2001. 2. Czoschke, N. M., M. Jang, and R. M. Kamens, Effect of acid seed on biogenic sceondary organic aerosol growth, Atmospheric Environment, In press. 3. Jang, M., S. Lee, and R. M. Kamens, Organic aerosol growth by acid-catalyzed heterogeneous reactions of octanal in a flow reactor, Atmospheric Environment, 37, 2125-2138, 2003. 4. Jang, M. S. and R. M Kamens, Atmospheric secondary aerosol formation by heterogeneous reactions of aldehydes in the presence of a sulfuric acid aerosol catalyst. Environmental Science and Technology, 35, 4758-4766,2001.

A42A MCC: Level 2 Thursday 1330h

Atmospheric Nitrogen Deposition to Critical Estuary Habitats: The Bay Regional Atmospheric Chemistry Experiment (BRACE) I Posters *(joint with B, OS)*

Presiding: **T B Watson,** NOAA Air Resources Laboratory**; N Poor,** College of Public Health, University of South Florida

A42A-0739 1330h POSTER

Partitioning of Nitric Acid to Nitrate by NaCl and $CaCO_3$ and Its Effect on Nitrogen Deposition

Melissa C. Evans[1] (813-974-5291; meevans@hsc.usf.edu)

Scott W. Campbell[2] (813-974-3907; campbell@eng.usf.edu)

Noreen D. Poor[1] (813-974-8144; npoor@hsc.usf.edu)

[1]University of South Florida, 13201 Bruce B. Downs Blvd. MDC 56, Tampa, FL 33612, United States

[2]University of South Florida, 4202 E. Fowler Ave. ENB 118, Tampa, FL 33620, United States

Nitrogen oxides produced by combustion in automobile engines, power plant boilers, and industrial processes are transformed to nitric acid in the atmosphere. This nitric acid then deposits to land or water and may be a significant nitrogen input to sensitive coastal estuaries. The sodium chloride from sea salt spray and calcium carbonate from mineral dust react in the atmosphere with nitric acid to form sodium nitrate or calcium nitrate, respectively. The nitrate particle deposition velocity can be substantially lower than that of nitric acid, which may lower the atmospheric nitrogen deposition rate near the urban sources of nitrogen oxides but raise the deposition rate over the open water. The relative effects of different ambient air concentrations of sodium chloride and calcium carbonate on nitrogen atmospheric deposition rates were examined by using the EQUISOLVII model to estimate the partitioning of nitric acid to nitrate combined with the NOAA buoy model and Williams model to calculate the gas and aerosol deposition velocities.

A42A-0740 1330h POSTER

Nitrate Aerosol Partitioning in the 2003 Bay Regional Atmospheric Chemistry Experiment (BRACE) : Aloft and Surface Comparisons

J. R. Arnold[1] (206.553.8579; jra@hpcc.epa.gov)

W. T. Luke[2] (301.713.0971; winston.luke@noaa.gov)

T. B. Watson[3] (208.526.9513; tom.watson@noaa.gov)

[1]NOAA/ARL Atmospheric Sciences Modeling Division on assignment to USEPA/ORD-NERL, 1200 6th Avenue 9th FL / OEA-095, Seattle, WA 98101-1128, United States

[2]NOAA/ARL Headquarters Division, 1315 East-West Highway, Silver Spring, MD 20910-6233, United States

[3]NOAA/ARL Field Research Division, 1750 Foote Drive, Idaho Fall, ID 83402, United States

The Bay Regional Atmospheric Chemistry Experiment (BRACE) field intensive in May 2003 was designed to help understand nitrogen chemistry and cycling in the airshed of Tampa, FL and included gas-phase and aerosol measurements at two downwind urban locations (Sydney and Tower Dairy) and a bay shoreline location (Gandy) as well as aboard the NOAA Twin Otter aircraft. The Twin Otter made 21 flights in the greater Tampa region over urban, suburban, and rural areas, Tampa Bay, and the Gulf of Mexico. Among these flights were several vertical profiles extending from 60 to 3000 m MSL over the Bay, the Gulf, and the ground sites. Aerosol samples on the Twin Otter were made with high flow rate filter packs followed by IC analysis; surface measurements for aerosols were made with a combination of filter packs, MOUDI samplers, annular denuders, and near-real time wet denuder collection followed by IC analysis. The degree of nitrate partitioning observed with the Twin Otter filter pack samples onto fine (2.5u and smaller) and large aerosols is examined separately for the three flow regimes that predominated during the intensive: strong synoptic, when local effects were overwhelmed; synoptic shift,

with wind shifts due to changing synoptic features; and sea/bay breeze, when local effects of the sea and bay breeze forced wind shifts. Analysis of these aloft results are then compared with nitrate aerosol values on the ground.

A42A-0741 1330h POSTER

Determination of the Boundary Layer Characteristics in the Tampa Bay Area During the Bay Region Atmospheric Chemistry Experiment (BRACE)

Ruth Laureen Gunter[1] ((865) 576-1246; gunter@atdd.noaa.gov)

Thomas B Watson[2] (Tom.Watson@noaa.gov)

Winston T Luke[3] (Winston.Luke@noaa.gov)

Jeff R Arnold[4] (Arnold.Jeff@epamail.epa.gov)

Clark W King[5] (Clark.W.King@noaa.gov)

[1]NOAA/ARL/ATDD, P.O. BOX 2456, Oak Ridge, TN 37830, United States

[2]NOAA/ARL/FRD, 1750 Foote Dr, Idaho Falls, ID 83402, United States

[3]NOAA/ARL/HQ, 1315 East-West Highway, Silver Spring, MD 20910, United States

[4]NOAA/ARL/AMD-USEPA, 4930 Old Page Rd, RTP, NC 27711, United States

[5]NOAA/ETL, 325 Broadway, Boulder, CO 80305, United States

Variability in boundary layer structure is to be expected in a coastal environment. It is necessary to determine the regional structure of the boundary layer to relate the chemical concentrations upwind and downwind of the urban area and to account for differences in the vertical concentration structure. NOAA's Air Resources Laboratory, using the NOAA Twin Otter, made meteorological and chemical measurements during 21 flights in and around the Tampa Bay area as part of the Bay Region Atmospheric Chemistry Experiment (BRACE). One or more vertical profiles were flown during each flight. The profiles were made from approximately 60 to 3000 m (200 to 10,000 ft) MSL, both over land and over the Gulf of Mexico. NOAA's Environmental Technology Laboratory (ETL) deployed three surface-based 915-MHz radar wind profilers equipped with radio acoustic sounding systems (RASS) during the experiment. The wind profiler/RASS systems were installed at Ruskin, Sydney and St Petersburg. The National Weather Service Office in Tampa (NWS/TBW) also released rawinsondes twice daily from the Ruskin site. The measurements of temperature, dew point, potential temperature, wind speed, and wind direction acquired during the aircraft profiles are analyzed and compared with the profiler and sounding data in order to determine the structure of the boundary layer over the Tampa Bay region and the temporal and spatial changes that occurred in that structure during the flights.

A42A-0742 1330h POSTER

Fast GC-Luminol Instrument for PAN and Nitrogen Dioxide Measurements

Nancy A. Marley[1] (marley@anl.gov)

Jeffrey S. Gaffney[1] (6302525178; gaffney@anl.gov)

[1]Argonne National Laboratory, Bldg. 203/ER, Argonne, IL 60439, United States

Fast gas chromatography (GC) with luminol detection was used to determine nitrogen dioxide and peroxyacetyl nitrate (PAN) levels onboard the National Oceanic and Atmospheric Administration Twin Otter during the Bay Region Atmospheric Chemistry Experiment (BRACE) in Tampa, Florida, in May 2002. Nitrogen dioxide concentrations measured by the fast GC-luminol technique were compared with simultaneous onboard NO2 determinations made by photolytic conversion to NO with subsequent ozone chemiluminescence detection. Use of photon counting (Hamamatsu HC-135) and an automated gas sampling valve enabled PAN measurement at 30-sec intervals. The fast GC-luminol system with photon counting will be described briefly. We recently improved the instrument and modified the outflow of the luminol carrier gas to minimize luminol spillage. Results will be presented for PAN during BRACE, and calibration data will be shown for the latest version of the instrument. The potential for luminol modification to improve sensitivity to PAN will also be discussed. This work was supported by the U.S. Department of Energy's Atmospheric Science Program.

A42A-0743 1330h POSTER

Heat Fluxes in Tampa Bay, FL

Kristin L. Sopkin[1] (727-553-1528; ksopkin@seas.marine.usf.edu); Mark E. Luther[1] (727-553-1528; luther@seas.marine.usf.edu); Sherryl A. Gilbert[1] (727-553-1036; sgilbert@marine.usf.edu); Vembu Subramanian[1] (727-553-1625; vembu@seas.marine.usf.edu); Jeff Scudder[1] (727-553-1337; jscudder@seas.marine.usf.edu); Lauren M. Wetzell[1] (727-553-1036; lwetzell@seas.marine.usf.edu)

[1]University of South Florida College of Marine Science, 140 7th Ave. South, St. Petersburg, FL 33701, United States

For the period of May 2002 to present, as part of the Bay Regional Atmospheric Chemistry Experiment, an observational tower has been maintained in Middle Tampa Bay that is equipped with sensors measuring meteorological and air-water turbulent flux parameters. Data acquired from this tower include air temperature, humidity and horizontal wind velocity measured at two heights, precipitation, incoming radiation, and barometric pressure. A SeaGauge sensor monitors water temperature, salinity, and water level, and a sonic anemometer measures the three-dimensional wind speed and the turbulent flux of momentum and sensible heat. Using data gathered from the tower, sea surface albedo and upwelling and downwelling long- and shortwave radiation fluxes are determined. Heat flux due to precipitation is calculated and the directly measured sensible heat flux is compared with the sensible flux derived using bulk formula and gradient-flux methods. Latent heat flux is also computed via the latter two methods. Temporal and vertical variations, including trends connected with seasonal and shorter signal scale events, are examined. Components of the heat budget of Tampa Bay are determined through a variety of pathways in order to constrain the error associated with the calculation of these parameters.

A42A-0744 1330h POSTER

Nitrogen Deposition to the Tampa Bay Watershed

Noreen Poor[1] (npoor@hsc.usf.edu); Paul Tate[1] (ptate@hsc.usf.edu); Mubeena Begum[1] (mbegum@hsc.usf.edu); Melissa Evans[1] (mevans@hsc.usf.edu); Scott Campbell[2] (campbell@eng.usf.edu); Venkat Bhethanabotla[2] (venkat@eng.usf.edu); Chris Bollinger[2] (spacepiper1@aol.com); Andrew Ball[2] (asball@eng.usf.edu)

[1]USF College of Public Health, 13201 Bruce B. Downs Blvd, Tampa, FL 33612, United States

[2]USF College of Engineering, 4202 E. Fowler Ave, Tampa, FL 33620, United States

An earlier estimate of the direct deposition of nitrogen to Tampa Bay was 7 kg-N/ha/yr and included the wet deposition of rainfall nitrate and ammonium and the dry deposition of nitric acid, ammonia, nitrate and ammonium. Rainfall and ambient air concentration measurements were made at an urban site within 50 m of Tampa Bay. Rainfall samples were obtained daily from a wet-only precipitation collector, which was part of the NADP AIRMoN. Ambient air concentrations of gases and fine particles were determined from an annular denuder system, operated at 10 l/min for 24-hr/day on a 1-in-6 day schedule, and dry deposition velocities were calculated with the NOAA buoy model using over water meteorological data. This estimate is revised upward to 8 kg-N/ha/yr and includes corrections for nitric acid collection inefficiencies, the addition of coarse particle nitrate based on mircoorfice impactor measurements, and improved fine and coarse particle deposition velocity estimates from an integrated NOAA buoy/Williams model. With gas, fine aerosol and coarse particle measurements made at a peri-suburban site coupled with deposition velocities from a resistance model, and rainfall concentration measurements from a rural NADP NTN site in Sarasota County, the estimated total nitrogen deposition to the surface of the watershed is 16 kg-N/ha/yr. The ratios of dry to wet deposition rates are 1:1 over water and 4:1 over land.

A42A-0745 1330h POSTER

Organic Composition of PM2.5 and Size-Segregated Aerosols During the 2002 Bay Regional Atmospheric Chemistry Experiment (BRACE), Florida, USA

Raphael T Tremblay[1] (rtremblay@rsmas.miami.edu)

Rod G Zika[1] (rzika@rsmas.miami.edu)

[1]University of Miami, Rosenstiel School of Marine and Atmospheric Science, 4600 Rickenbacker Causeway, Miami, Fl 33149, United States

Aerosol samples were collected for the analysis of organic source markers using a Tisch Environmental PM2.5 high volume sampler and two Micro Orifice Uniform Deposit Impactors (MOUDIs) as part of the Bay Regional Atmospheric Chemistry Experiment (BRACE) in Tampa, Florida. PM2.5 samples were collected at ground level on quartz fiber filters (QFF) while size-segregated samples were collected 12 meter above ground level on aluminum foil discs. MOUDIs with aerodynamic cut diameters of 18, 10, 5.6, 3.2, 1.8, 1.0, 0.56, 0.32 and 0.17 um were used. Samples were collected on a 24 hour schedule. The collected samples were solvent extracted using a mixture of dichloromethane/acetone/hexane, concentrated and then analyzed using a gas chromatograph/mass spectrometer (GC/MS) operated in single ion mode. PM2.5 extracts were analyzed using conventional splitless low volume injections (1 ul). Size-segregated aerosol extracts were analyzed using a Hewlett-Packard Programmable Temperature Vaporizing inlet (PTV) combined with large volume injections (80ul). Excellent chromatographic resolutions were obtained with either a 30 or 60 meter long RTX-5MS, 0.25 mm I.D. column. Target compounds were chosen to cover the range of potential sources and included alkanes and polycyclic aromatic hydrocarbons (PAH). Investigation of potential aerosol sources for different particle sizes using known organic markers and source profiles will be presented. Relationship between the collected PM2.5 and size-segregated samples will be studied. Size distributions of carbon preference indices (CPI), percent wax n-alkanes (%WNA) and concentration of selected compounds will be discussed.

A42A-0746 1330h POSTER

Spatial and Temporal Changes in Air Pollution Along the Gulf Coast Observed During BRACE: A Case Study of the Land-Sea Breeze

Dennis Wellman[1] (Dennis.L.Wellman@noaa.gov)

Winston Luke[1] ((301) 713-0971; Winston.Luke@noaa.gov)

Jeff Arnold[1] (Arnold.Jeff@epamail.epa.gov)

Tom Watson[1] (Tom.Watson@noaa.gov)

Laureen Gunter[1] (gunter@atdd.noaa.gov)

[1]NOAA/Air Resources Laboratory, NOAA/ARL(R/ARL) SSMC3, Rm. 3316 1315 East West Hwy., Silver Spring, MD 20910, United States

NOAA's Air Resources Laboratory conducted airborne measurements of trace gases and aerosols in the Bay Region Atmospheric Chemistry Experiment (BRACE) using the NOAA Twin Otter. The Twin Otter flew more than 90 hours in 21 flights in and around the Tampa metropolitan region in May, 2002, at altitudes of 60-3000 m MSL. Flights were conducted over rural and suburban areas, over the centers of Tampa and St. Petersburg, and over Tampa Bay and the Gulf of Mexico. One objective of the aircraft flights was to investigate the role of the sea breeze circulation in determining patterns of nutrient deposition and pollutant loads in the Tampa Bay watershed. Results will be presented from a May 8 flight designed to investigate the effect of the sea breeze recirculation upon Tampa's air quality. The Twin Otter took off at 1425 UTC and after performing a spiral ascent over the Sydney ground site, proceeded to fly north, at 200 feet above mean sea level (MSL) just off the Gulf coast, west of St. Petersburg. Back trajectory analysis suggested the dominance of a northerly rotation in the sea breeze; thus, air sampled over the Gulf passed some hours earlier to the south of the Tampa metropolitan area, in an area largely devoid of major pollution sources, before being advected eastward in the afternoon return flow. Ozone levels in this air mass ranged from 40 to 50 ppbv. Farther north the Twin Otter encountered the advected urban plume from Tampa, displaced to the north by the combination of southeasterly sea breeze flow and westerly return flow, and tracked this plume inland. Ozone levels quickly jumped to 60 ppbv, and increased to as high as 90 ppbv as photochemical processing continued in the advected plume. Nitric acid levels, which approached 4 ppbv in the aged urban air at the coast, dropped rapidly to as low as 1 ppbv inland. A final flight leg to the east of downtown Tampa encountered fresh anthropogenic pollution from the afternoon rush hour; ozone was rapidly produced in the brief transit time from emission to sampling by the aircraft. Analysis of the data will focus on the efficiency and rate of photochemical ozone production in the clean air, aged polluted airmass, and fresh pollution, and on the attendant extent of NOX oxidation and NOY loss.

A

A42A-0747 1330h POSTER

Prediction of Coarse Particle Nitrate From Fine Particle Measurements in a Coastal Environment

Scott W Campbell[1] (813-974-3907; campbell@eng.usf.edu)

Melissa C Evans[2] (meevans@hsc.usf.edu)

Noreen D Poor[2] (npoor@hsc.usf.edu)

[1]University of South Florida, College of Engineering 4202 E. Fowler Ave., Tampa, FL 33620, United States

[2]University of South Florida, College of Public Health 13201 Bruce B. Downs Blvd., Tampa, FL 33612, United States

Nutrient induced algal growth is one cause of decreased seagrass in the Tampa Bay Estuary. This influx of nutrients arises from the presence of fixed nitrogen in various flows and discharges to the estuary and from atmospheric deposition. One of the goals of BRACE (Bay Regional Atmospheric Chemistry Experiment) is to obtain improved estimates of the atmospheric nitrogen deposition to Tampa Bay. Previous estimates of atmospheric dry deposition of nitrogen to Tampa Bay have been based on Annular Denuder System (ADS) measurements of gaseous nitric acid and ammonia and fine particle (PM2.5) nitrate and ammonium, which extend back to 1996. However, recent coarse particle measurements indicate that, while ammonium primarily exists in fine particles, nitrate is preferentially found in the coarse fraction. The goal of this study is to examine whether the historical data for fine particle nitrate can be used to predict the amount of nitrate in the coarse fraction so as to obtain a more accurate estimate of dry particle deposition of nitrate to the Tampa Bay Estuary. Specifically, it is shown that averaged nitrate distributions obtained from recent micro-orifice impactor data can be used to predict the coarse to fine ratios observed for dichotomous samplers and the fine particle concentrations obtained from the Annular Denuder System. This provides some confidence that the impactor results may be used in conjunction with earlier fine particle data to obtain an estimate of coarse particle nitrate concentrations, and therefore an improved estimate of nitrate flux to the estuary.

A42A-0748 1330h POSTER

Ammonia Flux at the Air-Water Interface of Tampa Bay

Connie A. Mizak[1] (cmizak@hsc.usf.edu)

Noreen D. Poor[1] (npoor@hsc.usf.edu)

[1]University of South Florida College of Public Health, 13201 Bruce B. Downs Blvd., Tampa, FL 33612, United States

Recent nitrogen deposition research in the Tampa Bay Estuary indicates that ammonia deposition dominates the total dry nitrogen flux to the bay. Gaseous plus aerosol ammonia contribute approximately 450 tons per year or 60% of the total nitrogen deposition of 760 tons per year to the estuary. Research data also indicate that during the summer months, Tampa Bay may act as a source for atmospheric ammonia as water temperature and ammonium concentrations increase. Ammonia flux estimates will be derived from thirty days of daily summer air and water sampling at the Gandy Bridge air monitoring site located adjacent to Tampa Bay. Ammonia concentrations were measured at two heights with a URG, Inc. dual-pump annular denuder system (ADS), and water grab samples from two depths were analyzed in the laboratory for ammonium concentration. Hourly relative humidity, air and water temperature, pH and salinity were recorded at this site, and hourly wind speed and direction were obtained from the Environmental Protection Commission of Hillsborough County. Rainwater samples were obtained with a University of Michigan sequential rainwater collector and analyzed in the laboratory for ammonium concentration. The direction and magnitude for the ammonia flux will be calculated with a modified NOAA buoy model from measurements of wind speed, air and water temperature, air and water ammonia and ammonium concentrations, relative humidity, water pH and salinity. The results of this research will be used to improve the NOAA Buoy model, and to compare observed with modeled ammonia gradients.

A42A-0749 1330h POSTER

Simulation of Coarse Particle Nitrate Formations in Coastal Areas Using CMAQ-AIM

Ke Max Zhang[1] (1-530-754-8584; maxzhang@ucdavis.edu)

Robin L. Dennis[2] (1-919-541-2870; dennis.robin@epamail.epa.gov)

Michelle R. Mebust[2] (1-919-541-0833; mmebust@hpcc.epa.gov)

Prakash V. Bhave[2] (1-919-541-2194; bhave.prakash@epa.gov)

Anthony S. Wexler[3] (1-530-754-6558; aswexler@ucdavis.edu)

[1]University of California, Department of Mechanical and Aeronautical Engineering, University of California, Davis, CA 95616, United States

[2]National Oceanic and Atmospheric Administration, Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, Air Resources Laboratory, RTP, NC 27711, United States

[3]University of California, Department of Mechanical and Aeronautical Engineering, Department of Civil and Environmental Engineering and Department of Land, Air, and Water Resources, University of California, Davis, CA 95616, United States

The air quality model, CMAQ-AIM, was used to simulate the formation of coarse particle nitrate in coastal areas. CMAQ-AIM adopts USEPA's Models-3/CMAQ as the host photochemical model and employs a mechanistic, fully dynamic, internally-mixed, sectional aerosol module containing twelve aerosol species in nine size sections spanning 0.03 to 20 μm. The model's superior computational efficiency is achieved by a novel integration scheme and acid-neutrality gas-particle transport mechanisms, among which the Replacement Transport mechanism is particularly suitable for simulating the displacement of hydrochloric acid by nitric acid, or vice versa. The modeling results in Tampa Bay area from June 30 to July 14, 1999 episode (with sea-salt emission) in USEPA's Lower 49 State domain were compared to those produced by Models-3/CMAQ (without sea-salt emissions and a modal representation of the particulate matter). The preliminary comparison showed that total nitrate concentrations (gas and particle phase) were compatible between the two models, but CMAQ-AIM predicted a higher fraction of total nitrate partitioned into particle phase with over ninety percent of particle nitrate mass (about 1 μgm^{-3}) in the coarse mode, while fine particle nitrate mass was in the similar magnitude as accumulation mode particle nitrate simulated by Models-3/CMAQ. Due to CMAQ-AIM's ability to simulate sea salt and the displacement reaction, the importance of sea-salt emission in ambient air quality in coastal areas was demonstrated. Given that gas-phase nitrate deposition is usually reduced over water surface compared to that over land and coarse particle nitrate deposition remains unchanged, with high deposition velocity, our simulation indicates direct atmospheric particle nitrate deposition may significantly contribute to the total nitrate deposition into estuary habitats, which is consistent with BRACE measurement results. Since CMAQ-AIM also predicted coarse particle nitrate formation in many other coastal regions, our study suggests coarse mode nitrate needs to be measured in field campaigns in those areas; otherwise, a major fraction of total nitrate deposition would be missed.

A42B MCC: Level 2 Thursday 1330h

Ocean/Atmosphere Modeling I Posters *(joint with OS, NG)*

Presiding: **A Wallcraft,** Naval Research Laboratory**; L P Davis,** DOD High Performance Computing Modernization Program

A42B-0750 1330h POSTER

Development of Adaptive Mesh Refinement Techniques for an Ocean General Circulation Model

Aaron Herrnstein[1,2] (925-423-1971; aherrnst@llnl.gov)

[1]Institute For Scientific Computing Research, Lawrence Livermore National Laboratory, P.O. Box 808,, Livermore, CA 94551, United States

[2]Department of Applied Science, University of California at Davis, 3001 Engineering III 1 Shields Avenue, Davis, CA 95616-8254, United States

A problem faced by all computational physicists is the trade off between run time and grid resolution. The number of time steps and cost per time step drastically increases as finer and finer grids are used. In effort to combat this dilemma, research areas such as fluid dynamics use a modeling technique known as Adaptive Mesh Refinement (AMR). This involves increasing grid resolution in localized areas of the domain while preserving the structured nature of the original grid. The concept of AMR has been around for nearly two decades, but only in recent years have software packages become available to aid in many of the details. Atmospheric and ocean models simulate phenomena with motion derived from fluid dynamics. This suggests AMR is feasible for global climate modeling. The success of nested regional models also supports this hypothesis. In this research, techniques are developed which will allow AMR to perform on an existing ocean model known as the Modular Ocean Model (MOM). Of particular interest is the ability to use AMR on a staggered grid with centered differencing numerics. These are two characteristics of MOM which reduce computational noise and run time respectively. To aid AMR implementation, the software package SAMRAI (Structured Adaptive Mesh Refinement Application Infrastructure) is used. Refinement is based on solution gradients and possibly other criteria as needed. In addition, regions of critical topography might be refined if necessary. Current tools include time integrators which implement Leap Frog, Predictor Corrector, and Runge Kutta numerics. Velocities are defined at nodes and all other quantities at cell centers. A bench mark simulation of a barotropic modon will be presented.

A42B-0751 1330h POSTER

A Coupled Regional Climate Simulator for the Gulf of St. Lawrence, Canada

Manon Faucher[1] (514-282-6464, #253; manon.faucher@ec.gc.ca)

Francois Saucier[2] (418-775-0791; saucierf@dfo-mpo.gc.ca)

Daniel Caya[3] (514-282-6464, #340; caya.daniel@ouranos.ca)

[1]Meteorological Service of Canada / OURANOS, 550 Sherbrooke West, 19 floor (West tower), Montreal, Qc H3A 1B9, Canada

[2]Maurice-Lamontagne Institute, Department of Fisheries and Oceans, 850, Route de la Mer, Mont-Joli, Qc G5H 3Z4, Canada

[3]OURANOS, 550 Sherbrooke West, 19 floor (West tower), Montreal, Qc H3A 1B9, Canada

The climate of Eastern Canada is characterized by atmosphere-ocean-ice interactions due to the closeness of the North Atlantic Ocean and the Labrador Sea. Also, there are three relatively large inner basins: the Gulf of St-Lawrence, the Hudson Bay / Hudson Strait / Foxe Basin system and the Great Lakes, influencing the evolution of weather systems and therefore the regional climate. These basins are characterized by irregular coastlines and variables sea-ice in winter, so that the interactions between the atmosphere and the ocean are more complex. There are coupled general circulation models (GCMs) that are available to study the climate of Eastern Canada, but their resolution (near 350km) is to low to resolve the details of the regional climate of this area and to provide valuable information for climate impact studies. The goal of this work is to develop a coupled regional climate simulator for Eastern Canada to study the climate and its variability, necessary to assess the future climate in a double CO2 situation. An off-line coupling strategy through the interacting fields is used to link the Canadian Regional Climate Model developed at the "Université du Québec àMontréal" (CRCM, Caya and Laprise 1999) to the Gulf of St. Lawrence ocean model developed at the "Institut Maurice-Lamontagne" (GOM, Saucier et al. 2002). This strategy involves running both simulators separately and alternatively, using variables from the other simulator to supply the needed forcing fields every day. We present the results of a first series of seasonal simulations performed with this system to show the ability of our climate simulator to reproduce the known characteristics of the regional circulation such as mesoscale oceanic features, fronts and sea-ice. The simulations were done for the period from December 1st, 1989 to March 31st, 1990. The results are compared with those of previous uncoupled runs (Faucher et al. 2003) and with observations.

A42B-0752 1330h POSTER

Mountain Waves Forced by Narrow Topography in the Presence of Vertical Shear

James D. Doyle[1] ((831) 656-4716; doyle@nrlmry.navy.mil)

Qingfang Jiang[2] ((831) 656-4756; jiang@nrlmry.navy.mil)

[1]Naval Research Laboratory, 7 Grace Hopper Avenue, Monterey, CA 93943-5502, United States

[2]UCAR, 7 Grace Hopper Avenue, Monterey, CA 93943-5502, United States

The Alps is famous for its highly three-dimensional topography that features numerous narrow peaks over 3500 m, deep valleys, and steep mountain slopes. Three research aircraft were deployed to observe modest-amplitude gravity waves over the southwestern French