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AIRPACT: A REAL-TIME AIR QUALITY FORECAST SYSTEM

1. INTRODUCTION

a. Background

With the goals of promoting the use of innovative technology for developing environmental information and providing that environmental information to the public in a timely manner, the U.S. Environmental Protection Agency established the Environmental Monitoring for Public Access and Community Tracking (EMPACT) Program in 1998. The EMPACT Program works with communities via financial grants for projects that will make timely, accurate, and understandable environmental information available to millions of people in the largest metropolitan areas so that communities and individuals can make informed, day-to-day decisions about their lives. One such project, called the Air Indicator Report for Public Access and Community Tracking (AIRPACT), is underway in the greater Puget Sound Metropolitan Area of the State of Washington.

To increase public awareness of air quality issues in the Puget Sound region, and to promote changes in lifestyle to improve the region's air quality, EPA Region 10 (Seattle), the Washington Department of Ecology, and the Puget Sound Clean Air Agency are collaborating with the University of Washington and Washington State University in the AIRPACT project.

The intent of the Puget Sound AIRPACT program is to couple real-time air quality monitoring data with daily numerical forecasting of weather and air quality to provide the public, government agencies, other groups, and sensitive populations, with timely information regarding air guality. It will include the distribution of current and forecast air quality conditions to a wide audience through the web and regional media outlets as well as direct communication of air quality alerts to sensitive individuals through an Air Alert Hotline. In addition, AIRPACT will promote a better understanding of air quality issues in the Northwest and better science by facilitating regional development and evaluation of air quality modeling systems. By linking to the EPA AIRNOW program, AIRPACT will also contribute to the national knowledge base.

The motivation for developing a regional air quality simulation system for the Pacific Northwest and for the Puget Sound, in particular, arises from a history of periodic exceedances of the National Ambient Air Quality Standard (NAAQS) for ozone (Barna et al. 2000) and elevated levels of PM_{10} and $PM_{2.5}$. Although the region is currently in attainment of the ozone standard, past history suggests that the occurrence of high temperatures and stagnant winds can lead to elevated photochemical pollutant concentrations and possible exceedance of the NAAQS. Previous observational data and modeling results also indicate that a change in the ozone standard to 80 ppb (eight-hour average) would occasion additional future NAAQS violations.

In our recent development of a regional photochemical modeling system for the Cascadia region (Barna and Lamb, 2000), we employed the prognostic Mesoscale Meteorological Model Version 5 (MM5) (Dudia, Grell and Stauffer, 1994) to predict meteorological fields for this region of extremely complex terrain. The output from MM5 was re-formatted using the CALMET diagnostic model (Scire et al. 1995) in a mode where minimal changes to the MM5 winds were made. The resulting CALMET winds and boundary layer parameters were used as input to CALGRID, a state-ofthe art Eulerian photochemical air quality model (Yamartino et al. 1992). Hourly, gridded emissions data were compiled by the Washington Department of Ecology, and the modeling system was used to simulate an ozone episode that occurred during 11-14 July 1996. Results from this simulation showed that the modeling system demonstrated good performance in comparison to ozone observations at monitoring sites in the Puget Sound area and downwind of Portland, OR (Barna et al. 2000). Further analysis of this episode was completed where meteorological observations were incorporated into the MM5 solution using observational nudging (Barna and Lamb, 2000). In this case, model performance was improved compared to cases with no wind observations employed and with observations incorporated via interpolation using CALMET.

AIRPACT involves several components: 1) ongoing operation of an existing real-time air quality monitoring network and enhanced publication and distribution of hourly air quality data; 2) merging of existing MM5 daily weather forecasts and a gridded emissions inventory with a photochemical air quality model to produce detailed hourly maps of pollutant concentrations forecast 24 to 48 hours into the future; 3) implementation of an Air Quality Alert Hotline to families of children with asthma regarding forecast periods of poor air quality; and 4) public outreach and education to promote a clear understanding of the air quality data and forecasts through the Air Watch Program of the Puget Sound Clean Air Agency. The AIRPACT program plans to take advantage of a variety of media for dissemination of the daily air quality information including an established web site, transfer of information and useful graphics to the broadcast media and newspapers, and development of a direct communication air quality alert system for asthmatic children using automated phone systems. A variety of products ranging from charts of Air Quality Indices (AQI) to actual pollutant concentrations for ozone, PM_{2.5}, and PM₁₀, will insure that the public can access air quality information at an appropriately useful technical level.

The AIRPACT program seeks to exploit several technological resources available in the Puget Sound region to demonstrate the potential to educate and inform the public about air quality issues. The technological capital being leveraged in this effort includes:

- Expertise and computer infrastructure for meteorological modeling at the University of Washington, Department of Atmospheric Sciences,
- Expertise in emissions inventory preparation at the Washington Department of Ecology (Ecology, hereafter),
- Real-time air quality monitoring data from a multisite network operated by Ecology, and the Puget Sound Clean Air Agency (PSCAA)
- Expertise in air quality modeling at Washington State University, Department of Civil and Environmental Engineering.

The AIRPACT project can be summarized as the automated application of current state-of-the-art meteorological and air quality models to short term air quality forecasting, with feedback from an air quality sensor network, coupled with a public education program and a targeted outreach program for vulnerable populations. Whereas the AIRPACT air quality forecasting is highly automated, generating air quality prediction results by each morning for the day, decisions to issue air quality alerts are decided by meteorologists and public health experts and will not be automated for the foreseeable future. This paper presents the basics of the AIRPACT air quality forecasting system, with examples of emissions results and simulation results.

b. Domain

The AIRPACT domain is rendered as a Lambert Conformal projection grid bounded on the southwest corner by 46.07° N., 123.66° W and on the northeast corner by 48.54° N and 120.35° W, and is defined to be

13 layers in depth. The gridded domain is composed of 62 columns (E-W) by 67 rows (N-S) of 4-km cells. The domain (Figure 1) extends from the shoulders of the Olympic Mountains on the Olympic Peninsula in the west, eastward over the Puget Sound, past Mt. Rainier and into the middle of the Cascade Mountain Range in the east, and from near the Canadian border with Washington State in the north to the vicinity of Longview, Washington, and the mouth of the Columbia River in the south. The domain thus encompasses the Puget Sound, the major metropolitan areas of Seattle and Tacoma, and the north-south I-5 (interstate highway) corridor. The vertical coordinate system is the sigma system used in MM5, but MM5 layers have been combined to provide for 13 layers reaching an elevation of ~5 km. The sigma layer depths depend on local pressure; representative layer-top elevations (above the surface) are {20, 57, 95, 133, 209, 364, 521, 681, 925, 1346, 2152, 3133 and 4949} meters. This domain was selected based on results from earlier photochemical air quality simulations using a much larger domain (Barna et al. 2000; Barna and Lamb, 2000) that showed little transport of pollutants from the Vancouver, BC. Metropolitan area into the Puget Sound region. However, experience shows that the domain appropriate for a modeling application, such as AIRPACT, typically changes over time as policy requirements and/or computational and/or informational resources change. For this reason, the AIRPACT system automates the sharing of domain-specific information that must be universally available among AIRPACT system components. Thus, the fullest use of metadata defining the domain is a significant implementation detail throughout the system design.

ELEVATION

AIRPACT 4-km Domain



Figure 1. Map of AIRPACT modeling domain in western Washington.

2. AIRPACT SYSTEM

a. System Design for AIRPACT

As shown in Figure 2, the air quality forecasting system for AIRPACT utilizes MM5 meteorological forecasts. These forecasts are produced by running MM5, the Penn State Mesoscale Meteorological Model, version 5 (Dudhia, Grell and Stauffer, 1994), for a set of nested domains with grid spacings of 36-km, 12-km and 4-km, with the outermost 36-km model runs being initialized at 0000 UTC and 1200 UTC each day. AIRPACT currently uses forecast hours 12 through 36 from a 4-km simulation based on a 12-km MM5 run initialized at 1200 UTC. The CALMM5 and CALMET processors pass MM5 wind fields to CALGRID. Thus the CALGRID simulation begins at 4:00 AM PST. In processing MM5 hourly data, CALMM5 extracts temperature and short wave radiation fields that are then made available for emissions processing, as discussed in a subsequent Typical applications of CALMET/CALGRID section have been to examine historical ozone episodes of interest, such as the Puget Sound event of 11-14 July 1996 (Barna et al. 2000). In such applications, meteorological data from surface analyses and vertical soundings are used with CALMET. In the AIRPACT forecast application, however, no such data is available beyond the simulation results provided from MM5. Thus, AIRPACT seeks to maximize the utility of the MM5 data for producing useful CALMET results.

The version of CALGRID being used in AIRPACT employs the SAPRC97 chemistry mechanism (Carter, 1996; Carter, Luo and Malkina, 1997). Various enhancements are envisioned for the air quality forecasting system as shown in Figure 2. Not shown are enhancements to the preprocessing of MM5 data to increase the amount of boundary layer data available to CALGRID. Also, as indicated in the schematic of Figure 2, the option of extracting initial conditions for a subsequent CALGRID run has been developed, although it was not in use during the August simulation shown herein.

b. System Implementation

AIRPACT is built primarily of processors (CALMM5, CALMET and CALGRID) written in FORTRAN77. Visualization post-processing is being done (currently and experimentally) using the North Carolina Supercomputing Center's PAVE package; PAVE requires netCDF data files, which are generated using file conversion codes written in FORTRAN90. The automation of the AIRPACT system is accomplished using perl and cshell scripts. Performance on a University of Washington Compaq/DEC Alpha system for a single processor run is ~70 minutes for a 24 hour simulation.

c. Emissions Processing

Emissions preparation for the CALGRID run is a critical aspect of the AIRPACT forecasting system. CALGRID accepts emissions in various input files; AIRPACT utilizes emissions of four types: 1) mobile vehicle emissions, 2) area biogenic emissions, 3) point source emissions and 4) anthropogenic emissions treated as area (aggregates of small point sources). A schematic of the mobile emissions processing method is shown in Figure 3 and a similar diagram for biogenic emissions is shown in Figure 4.



Figure 2. AIRPACT air quality simulation system schematic. Processors are shown in boxes and files as cans.

Mobile Emissions Generation



Figure 3. Schematic of mobile emissions processing scheme.

Mobile emissions representing the vehicular sources of emissions are generated for each hour of CALGRID simulation. Two aspects warranting detailed discussion are the preparation of the base gridded mobile emissions inventory (with adjustment factors) and the run-time emissions preparations.

Vehicles generate emissions both through engine exhaust and through a variety of evaporative losses. These evaporative losses have been further identified as being of six types: hot soak, diurnal, crankcase, running, resting, and refueling. Ecology's treatment combines the first three into a single evaporative category, and relegates evaporative losses during refueling to anthropogenic area emissions (such as gas stations), resulting in four classes of vehicle emissions: EVAPORATIVE, EXHAUST, RESTING, and RUNNING. Ecology prepared the AIRPACT mobile emissions through a multi-step process.

- Using TIER2 software (based on MOBILE5B) representative vehicle fleet data corresponding to three types of areas were processed for emissions over a range of temperatures (Koupal and Rykowski, 1998; Koupal, 1999; Kremer, 1999). These simulations were performed for both summer and winter conditions, with fuel Reid Vapor Pressure (RVP) values of 7.8 and 12.8 p.s.i., respectively. (Summer RVP is controlled to be no greater than 9.0 p.s.i. by law in Washington.)
- 2. Base emission rates for 75° F for the three types of areas, for summer and Winter RVPs, were extracted from the TIER2 results.
- 3. The emission rates sensitivity for temperature was determined by analysis of the TIER2 results, for both summer and Winter RVP.
- January 2001 Vehicle Miles Traveled (VMT) estimations were obtained by updating data from 1994—1997, based on traffic projections by the Washington Department of Transportation and other local transportation planning agencies.
- 5. Road segment-based estimates for January 2001 VMT were regridded to a 5-km grid.
- Washington Department of Transportation data were used to develop weighting functions for time of day, day of week and month for levels of vehicular activity (VMT).
- Emissions (seasonal and area specific) were mapped to the gridded base VMT activity levels to obtain a gridded base emissions inventory by season representing a daily speciated emission inventory for a base day, with an implicit reference temperature of 75°F.

AIRPACT has chosen to produce a detailed mobile emissions inventory, as described in the steps above, to

support generation of highly realistic vehicle emissions throughout any simulation period. Thus, by using descriptions of temperature sensitivity and temporal variability, mobile emissions can be generated on an hourly basis, utilizing gridded MM5 surface layer temperatures, and reflecting observed temporal variability of traffic.

Biogenic emissions for AIRPACT have been generated using MM5 domain descriptor data and GLOBEIS, and hourly MM5 data (Figure 4). MM5 data for one hour of an April 2001 date were modified to fix temperature at 30C and short wave downward flux equivalent to PAR (Photosynthetically Active Radiation, a measure of photon flux) of 1000 μ Mol m⁻² s⁻¹. This MM5 data was then processed using GLOBEIS (Guenther et al. 2000), and the resulting hour of gridded emissions was then speciated to SAPRC97. These gridded biogenic emission results are then modified on a run-time basis using hourly, gridded temperatures and short wave downward flux from MM5, according to equations for isoprene and other VOCs from Guenther et al. (1993). Thus for each hour of CALGRID simulation, a base map of speciated biogenic emissions is modified for predicted temperature and light levels to project biogenic emissions for that hour.

Biogenic Emissions



Figure 4. AIRPACT process for calculating biogenic emissions.

Point emissions for AIRPACT are likewise constructed on an hourly basis for each AIRPACT CALGRID run. The basic point emissions inventory consists of a list of point sources with descriptive metadata, including the point location, constructed for a four-day period in July 1996, a Thursday through Sunday period. This inventory of point emitters is windowed to reject those points not found within the AIRPACT domain. Point emissions for all hours of this period are then recast into files for Weekday, Friday, Saturday and Sunday, each of 24 hours. These data are then read as required from these four single day files to construct a time sequence of hourly point emissions to match the days of the week and the hours required for the CALGRID run.

Anthropogenic area emissions are similarly constructed on an hourly basis for each run. The basic area emissions inventory consists of gridded hourly emissions for the 11-14 July 1996, a Thursday through Sunday period. This inventory is regridded, windowed, and recast into files for Weekday, Friday, Saturday and Sunday, each of 24 hours. These data are then read as required from these four single day files to construct a time sequence of hourly area emissions to match the days of the week and the hours required for the CALGRID run.



Figure 5. Emissions contour map for mobile NOX emissions during the afternoon rush hour.

An example of mobile NOX emissions is shown for 10 August 2001 in Figure 5, showing the domination of the Puget Sound mobile emissions by the Seattle metropolitan area and highway network. (PAVE tile plots shown herein display the hourly cell minimum and cell maximum values at the bottom of the figure.) Figure 6 shows the diurnal mobile emissions pattern with a rush hour peak in the 0600-0700 PST hour and a broader peak from 1500-1800 PST (The diurnal line plots shown report values for a 40 km by 100 km subdomain (21,28 to 30,52) containing the Seattle area.)

Biogenic Isoprene emissions for August 10 are shown in figures 7 and 8, the latter displaying a diurnal cycle that shows these emissions functional dependence on light and temperature. Area NOX emissions are shown in Figures 9 and 10, and show how area emissions reflect both population density and the diurnal cycle associated with work-day activity levels (August 10, 2001 was a Friday).



Figure 6. Diurnal pattern of mobile NOX emissions as average cell value [g/s/cell] for the Seattle area.

Biogenic Isoprene Emissions



Figure 7. Emissions contour map for biogenic isoprene emissions.



Figure 8. Diurnal pattern of biogenic isoprene emissions as average cell value [g/s/cell] for the Seattle area.



d. Simulation Results

CALGRID results are generated nightly with animations of selected emissions, concentrations and statistics being made available via a project web-site at **www.atmos.washington.edu/~empact/mm5aq.html**. CALGRID concentration forecasts for O3 and NOX for the 10 August 2001 simulation are shown in Figures 11, 12, 13 and 14 to illustrate typical results. The O3 pattern in Figure 11 shows a typical simulation result for warm summer days with northerly flow through the Puget Sound. Seattle area ozone peaks in the early afternoon (Figure 12) but the domain maximum occurs in the 1500-1600 PST period at cell (17,35) across the sound southwest from Seattle. The midday decrease in Seattle area NOX at 1300 PST (Figure 14) coincides with the area O3 maximum (Figure 12). Also, by 1600 PST the Seattle area appears to be dominated by a NOX plume (or pall) originating in area and mobile emissions. A second plume is visible in Figure 13 flagging southeasterly from a power plant location marked as CPP, in Lewis County.



Figure 10. Diurnal pattern of NOX area emissions as average cell value [g/s/cell] for the Seattle area.



Figure 11. Ozone simulation results for Puget Sound area. Seattle is marked as S.



Figure 12. Simulated diurnal pattern of ozone as average cell value [ppm] for the Seattle area.



Figure 13. NOX simulation results for Puget Sound area. The location of a power plant in Centralia, WA is marked as CPP.

e. Verification Using Surface and Airborne Sensors

AIRPACT simulation results are automatically compared (a day later) with air quality observations from an automated instrument network operated by Ecology. Mean bias and root mean square error statistics are computed for all available stations for O3, NO, NO2, and CO. Verification has only recently been implemented and although preliminary verification results appear to be both promising and useful, these are not presented here.

An additional source of data for model verification comes from an August 2001 NARSTO (North America Research Strategy for Tropospheric Ozone) aircraft study called PNW 2001 conducted collaboratively by the Pacific Northwest National Laboratory, EPA Region 10, the Washington State Department of Ecology, the University of Washington and Washington State University, in cooperation with the Canadian Pacific 2001 study. AIRPACT results will be evaluated using aircraft and ozonesonde data from PNW 2001.



Figure 14. Simulated diurnal pattern of NOX as average cell value [ppm] for the Seattle area.

3. CONCLUSION

a. System Feedbacks

Several aspects of the AIRPACT system promise to provide modelers with ample feedback, helping them to focus available resources on model skill, emissions accuracy or other science, code or data issues. For example, during the 10 August 2001 simulation shown here, gaps in roadways can be seen in the mobile emissions results in Figure 5; since this simulation the mobile emissions data have been updated to correct this problem. Also, strong area emissions for NOX have been detected in suspicious areas (Figure 9) and traced back to spatial allocation problems for marine (ship fuel combustion) emissions; the spatial allocation of marine emissions is being reviewed. Lastly, the blocky pattern visible in biogenic isoprene emissions suggests that our use of GLOBEIS results in relatively coarse-scale emissions, prompting a review of our biogenics processing. In general, AIRPACT's automated

animations and automated verification support the identification of desired corrections and enhancements.

Despite minor problems identified by exercising AIRPACT, this air quality simulation system is proving to be a unique tool to study the performance (accuracy) of the CALGRID air quality modeling with SAPRC97 chemistry, the correctness of the emissions subsystems and the adequacy of the associated emissions inventories. Evaluation of air quality forecast verification statistics with reference to categories of meteorological conditions can 1) help identify weak areas in the air quality modeling components, and 2) guide improvements to these models, or 3) motivate their replacement with another model, e.g. CMAQ.

b. Summary

The AIRPACT project is demonstrating a highly automated real-time air quality forecasting approach in application to the Puget Sound area. The AIRPACT design targets linkage of real-time monitoring to forecasting for purposes of verification and seeks to apply air quality modeling both to educate the public and to alert sensitive individuals to potentially dangerous pollution episodes. AIRPACT is operating with a full flow of emissions in a test mode and generating daily air quality forecasts for review.

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