Enhancement and evaluation of the AIRPACT ozone and PM$_{2.5}$ forecast system for the Pacific Northwest

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The Air Indicator Report for Public Access and Community Tracking (AIRPACT) real-time numerical air quality forecast system operates daily in the Pacific Northwest region to predict hourly ozone, PM$_{2.5}$ and related precursor and pollutant species. In an update to the existing AIRPACT forecast system, the MM5/SMOKE/CMAQ Eulerian modeling system replaces the MM5/CALMET/CALGRID model framework. The new system, AIRPACT-3, has a larger domain that encompasses Washington, Oregon, Idaho, and bordering areas. The system includes a highly dynamic emission processing subsystem which incorporates anthropogenic and biogenic emissions, as well as real-time wildfire emission estimates, and a dynamic daily ammonia emissions module. As an initial evaluation of the system, forecast results were compared against measurement data for the August–November 2004 period. Analyses showed that the system is skillful in predicting episodic ozone conditions (8-h daily maxima) above 50 ppbv, but systematically over-predicts levels less than 40 ppbv. For fine particulate matter, PM$_{2.5}$, the system captures the concentration differences between urban and rural regions, and captures qualitatively the specified distribution of fine PM$_{2.5}$ component concentrations. A separate emission sensitivity study shows the system can adequately simulate the PM pollution impacts from fire events; however, the new dairy ammonia emission module has lesser impact on the overall PM$_{2.5}$ forecast performance.


1. Introduction

Air pollutants, such as tropospheric ozone and particulate matter, can cause adverse health effects in humans and degrade ecosystem integrity. To protect the public health and welfare, the U.S. Environmental Protection Agency (EPA) established the National Ambient Air Quality Standards (NAAQS) for ozone (O$_3$) and particulate matter (PM) with aerodynamic diameters less than 10 µm (PM$_{10}$) and 2.5 µm (PM$_{2.5}$). Recently, with advances in computational technology, regional air quality forecast systems have shifted from analyses of forecast meteorology and statistical methods to the use of sophisticated computational numerical models that account for meteorology, emissions and chemistry simultaneously. Several such systems have been implemented around the world and in the U.S. Examples include: the Australian AAQFS (http://www.epa.vic.gov.au/air/aaqfs/), the Canadian CHRONOS [Pudykiewicz and Kozioł, 2001] (http://www.msc-smc.ec.gc.ca/aq_smog/chronos_e.cfm), the UK NAME-III system (http://www.airquality.co.uk), and, several systems in the eastern U.S. reviewed by McKeen et al. [2005]. Recently in the U.S., EPA and NOAA have begun development of a ETA-CMAQ numerical forecast system to predict ozone and wild-fire smoke pollutants for the conterminous U.S. [Otte et al., 2005]. The results from this numerical forecast are now part of the U.S. government public Internet resources for national air quality (http://www.weather.gov/aq/).

In the Pacific Northwest Region, as part of the Northwest International Air Quality Environment Science & Technology Consortium (NW-AIRQUEST, http://www.nwairquest.wsu.edu), the Air Indicator Report for Public Access and Community Tracking (AIRPACT) real-time numerical air quality forecast system, has been providing hourly air pollutant predictions since May 2001. The objective of the system is to provide additional information to aid state and local air quality managers in the identification of the onset of poor air quality conditions, and if necessary, issue warnings to the general public. The AIRPACT system (AIRPACT-1 [Vaughan et al., 2004] and AIRPACT-2 [Mahmud, 2005]) was originally based on the MM5/CALMET/CALGRID modeling framework and was primarily designed for ozone pollution prediction. Recently, the system was upgraded as AIRPACT-3 to include aerosol chemistry and fume via the EPA Community Multi-scale Air Quality (CMAQ) modeling system [Byun and Schere, 2006].

In this paper, we describe the AIRPACT-3 real-time air quality forecast system and present an initial evaluation...
of the forecast performance for ozone, total mass PM$_{2.5}$ and PM$_{2.5}$ components. The system was applied for a four-month period, August–November 2004. This period was chosen to encompass both summer ozone conditions and wintertime stagnant PM conditions and also to take advantage of additional PM observations from an intensive field campaign conducted in the vicinity of the Columbia River Gorge. Observational data for ozone and PM$_{2.5}$ were obtained from the EPA-AQS network and the IMPROVE PM speciation network as well as from a special measurement program conducted by the Southwest Clean Air Agency (SWCAA) in the Columbia River Gorge. This evaluation provides an important first look at the ability of the CMAQ system to simulate atmospheric chemical conditions with forecast emissions and meteorology in the Pacific Northwest. The following sections describe the forecast system framework, the evaluation process, and observational data used, and then results are presented in terms of pollution forecast performance.

2. Forecast System Description

2.1. Chemical Transport Model

The core photochemical transport model (CTM) in AIRPACT-3 is the CMAQ Chemical Transport Model (CCTM, version 4.6). The model accounts for chemical interactions for compounds in gas, aqueous and aerosol phases. The chemical mechanism applied in the model is the “saprac99 ae4_aq”, with the SAPRC99 gas-phase chemical mechanism [Carter, 2000] and aerosol module (version 4) that includes the ISORROPIA secondary inorganic aerosol algorithms [Nenes et al., 1998] and the SORGAM secondary organic aerosol formulations [Schell et al., 2001]. The aerosol module contains aerosol process dynamics for nucleation, coagulation, condensation, evaporation and dry deposition [Binkowski and Roselle, 2003]. Wet deposition of both aerosol and gas-phase compounds are included in cloud processes that scavenge chemical species via aqueous chemistry and attenuate incoming shortwave radiation that is important for photolytic reactions. Horizontal and vertical advection are calculated using the “YAMO” method [Hu et al., 2006] and the atmospheric turbulent diffusion is modeled with the K-theory eddy diffusion scheme.

Particle size distributions in CMAQ are represented via a modal approach with three overlapping lognormal aerosol size modes: Aitkin mode, accumulation mode and coarse mode. The distributions describe the modeled particle size ranges defined by their geometric mean diameters and geometric standard deviations. These parameters vary depending on the composition and density of the particle components in each mode. The fine particles in the Aitkin and accumulation modes interact with each other via coagulation. Particle chemical components are assumed to be internally mixed and at equilibrium. Particle chemistry, condensation, evaporation and deposition are modeled within each mode without intermodal interactions. Since CMAQ reports particle concentrations for the three lognormal distributions, the PMx program is used to post-process model output for size-resolved PM$_{2.5}$ mass concentrations for individual aerosol component species [Jiang et al., 2006].

2.2. Model Domain and Forecast Period

The AIRPACT-3 domain, shown in Figure 1, encompasses all of Washington, Oregon and Idaho along with portions of bordering states and Canadian provinces. The domain consists of 95 by 95 horizontal grids at 12 km grid
resolution. Vertically, there are 21 layers, with the bottom first layer at approximately 35 m above the surface.

In the configuration used for this evaluation, AIRPACT-3 provides a 24-h air quality forecast beginning at 8-h GMT (0-h PST) for the next day. The system is initiated daily at midnight and is able to complete the entire simulation and post processing in less than 4 h with graphical output available by approximately 4 am local time. Recently, the system was extended to provide 64-h forecasts, but these longer term forecasts are not considered in the evaluation presented here.

### 2.3. Meteorology

The forecast meteorology for AIRPACT-3 comes from the Mesoscale Meteorological model (MM5 version 3.7.3) [Grell et al., 1994] operated by Mass and colleagues at the University of Washington (http://www.atmos.washington.edu/mm5rt). The MM5 forecast system provides hourly, 3-D gridded meteorological variables over the Pacific Northwest region at 36-, 12-, and 4-km grid resolutions with 37 vertical levels for the next 48 to 72 h. For the work presented here, the AIRPACT-3 system uses the 12-km MM5 output initialized with the 00Z-h data from the National Center for Environmental Prediction (NCEP) GFS model results. Initialization with global forecast model driven by observations is necessary for forecast meteorology to keep the model from going astray over an extended simulation period. In the AIRPACT-3 system, the 00Z initialized MM5 outputs are spun-up for 8 h before being used in the CMAQ for air quality forecast. More information, including model configuration and overall performance, of the MM5 forecast simulations are discussed by [Mass et al., 2003] and on the University of Washington-MM5 website. The AIRPACT-3 system is initiated nightly after the meteorological results from MM5 become available.

### 2.4. Emissions

The AIRPACT-3 emission subsystem includes emission processing steps to generate gridded, hourly data that reflect the projected emission activity across the modeling domain. The subsystem is initiated daily to process emissions from four major categories: anthropogenic, biogenic, ammonia emissions from dairy operations, and wild fire emissions. Table 1 summarizes average emissions by source categories in the domain. Overall, the anthropogenic mobile sources represent the bulk of NOx emissions. VOC emissions for the modeling period are dominated by biogenic and fire sources. Fire events also produce significant amounts of primary PM emissions compared to anthropogenic sources.

#### 2.4.1. Anthropogenic Emissions

The Sparse Matrix Operator Kernel Emissions (SMOKE) model version 2.1 [Houyoux et al., 2000; Carolina Environment Programs, 2005] was modified to process anthropogenic emission categories for each forecast simulation. Area and nonroad mobile emissions are based on the 2002 EPA National Emission Inventory data set (available at http://www.epa.gov/ttn/chief/net/2002inventory.html) and adjusted to year 2005 with county and source specific projection factors from the EPA Economic Growth Analysis System (EGAS) software [U.S. EPA, 2006]. On-road mobile emissions are generated outside the SMOKE framework using emission factors from the EPA MOBILE v6.2 model [U.S. EPA, 2003] and the 2005 state specific activity data. Emissions are generated at a normalized temperature of 30°C such that adjustments for the evaporative loss emission fraction can be applied during each forecast simulation. The mobile emission temperature adjustment factors were region specific and generated from the MOBILE v6.2 model. Point source inventory is based on the same national data set with updates by the emissions workgroup within NW-AIRQUEST to reflect 2005 operation activities for Washington, Idaho and Oregon. Anthropogenic emissions over provinces of British Columbia and Alberta, Canada are included from a 2000 inventory [GVRD Canada, 2002].

The hourly distribution of emissions in SMOKE accounts for month, weekday/weekend/holiday activity differences by source categories for each simulation day. Mobile source emissions are adjusted with temperature dependent emission factors and the hourly forecast MM5 temperatures. Point source emissions are distributed vertically for active plume rise with MM5 forecast meteorology.

#### 2.4.2. Biogenic Emission

The BEIS3 (Biogenic Emissions Inventory System version 3) model, as part of the SMOKE processor, is used to estimate hourly biogenic emissions. The gridded 1-km BELD3 land use data set was preprocessed for normalized biogenic emissions for summer and winter biomass distributions. The seasonal normalized emissions are adjusted by

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### Table 1. Summary of Typical Week-Day Emission Inventory and August–November 2004 Monthly Fire Emissions Within the AIRPACT-3 Modeling Domain

<table>
<thead>
<tr>
<th>Category</th>
<th>CO</th>
<th>NOx</th>
<th>VOC</th>
<th>NH3</th>
<th>SO2</th>
<th>PM10</th>
<th>PM2.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anthropogenic emission, tons/d</td>
<td>14846</td>
<td>2465</td>
<td>3241</td>
<td>1306</td>
<td>631</td>
<td>2393</td>
<td>1014</td>
</tr>
<tr>
<td>Biogenic emission, tons/d</td>
<td>152</td>
<td>2082</td>
<td>5682</td>
<td>10378</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dairy operations in Washington and Oregon, tons/d</td>
<td>79</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire emission August, kilotons/month</td>
<td>1714</td>
<td>104</td>
<td>199</td>
<td>17</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire emission September, kilotons/month</td>
<td>71</td>
<td>7</td>
<td>7</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire emission October, kilotons/month</td>
<td>309</td>
<td>23</td>
<td>28</td>
<td>3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire emission November, kilotons/month</td>
<td>203</td>
<td>15</td>
<td>19</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1. OVOC does not include isoprene and terpenes.
Definitions of Model Performance Statistics

<table>
<thead>
<tr>
<th>Number of Paired Data Points</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean bias (MB)</td>
<td>$\frac{1}{N} \sum_{i=1}^{N} (M_i - O_i)$</td>
</tr>
<tr>
<td>Mean error (ME)</td>
<td>$\frac{1}{N} \sum_{i=1}^{N}</td>
</tr>
<tr>
<td>Predicted mean ($\bar{M}$)</td>
<td>$\frac{1}{N} \sum_{i=1}^{N} M_i$</td>
</tr>
<tr>
<td>Measured mean ($\bar{O}$)</td>
<td>$\frac{1}{N} \sum_{i=1}^{N} O_i$</td>
</tr>
<tr>
<td>Normalized mean bias (NMB), %</td>
<td>$\frac{1}{O_i} \sum_{i=1}^{N} (M_i - O_i)$</td>
</tr>
<tr>
<td>Normalized mean error (MBE), %</td>
<td>$\frac{1}{O_i} \sum_{i=1}^{N}</td>
</tr>
<tr>
<td>Fractional bias (FB), %</td>
<td>$\frac{1}{(M_i + O_i)} \left( \frac{M_i - O_i}{0.5(M_i + O_i)} \right)$</td>
</tr>
<tr>
<td>Fractional error (FE), %</td>
<td>$\frac{1}{(M_i + O_i)} \left( \frac{</td>
</tr>
<tr>
<td>Correlation coefficient ($r$)</td>
<td>$\frac{\sum_{i=1}^{N} (M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^{N} (M_i - \bar{M})^2 \sum_{i=1}^{N} (O_i - \bar{O})^2}}$</td>
</tr>
</tbody>
</table>

$M_i$ – Predicted concentration, $O_i$ – measured concentration

grid for each simulation day with forecast hourly temperature and shortwave radiation.

2.4.3. Ammonia Emissions

Gas-phase ammonia in the atmosphere plays an important role in the formation of secondary inorganic aerosol [Pinder et al., 2006]. In the Pacific Northwest, livestock facilities produce large quantities of ammonia [Rumburg et al., 2004, 2006]. The AIRPACT-3 system contains a new dairy ammonia emissions module based upon empirical algorithms from measurements [Rumburg, 2006]. The module incorporates emissions for three types of dairy operations: animal housing, manure storage and manure processing. In the current model implementation, ammonia emissions are estimated for each individual dairy with site specific input parameters provided by Oregon and Washington state agencies. The module is executed for every forecast simulation, and the algorithms adjust ammonia emissions with forecast hourly temperature and wind speed.

In the current setup, due to a lack of specific dairy information, ammonia emissions for Idaho and other areas were taken from the EPA national inventory data set and processed in SMOKE. Ammonia emissions from other sources such as fertilizer application, feedlot operations and industrial activities are included and processed as part of the anthropogenic inventory.

2.4. Wild Fire Emission

Large scale fires contribute significant amounts of pollutants and pollutant precursors to the atmosphere [Miranda, 2004; Malm et al., 2004]. AIRPACT-3 incorporates forecast fire emissions via direct interface with the USDA-Forest Service BlueSky smoke modeling system (http://www.BlueSkyRains.org) [O’Neill et al., 2006a]. Each day, the BlueSky system estimates fire emissions by location with fire event data from the National Interagency Fire Center. Output from the BlueSky model contains CO, total organic carbon (TOC), primary PM$_{2.5}$ and coarse PM (PMC) emission as well as fire area and heat flux estimates for each individual fire. Fire emissions are treated as individual point sources at reported locations. The emissions are allocated to vertical layers using the buoyant plume rise algorithm with the estimated heat flux. Each day, the AIRPACT-3 system retrieves the fire information and incorporates the data as part of the emission input to the CMAQ model.

There is extensive agricultural field burning within eastern Washington and northern Idaho, and these sources are currently managed using the ClearSky smoke dispersion forecast system (http://www.cleasky.wsu.edu) [Jain et al., 2007]. However, currently the emissions from these burns are not included in AIRPACT-3 primarily because the burn managers in the region consider a wide range of burn scenarios and, thus, it is difficult to specify an accurate acreage forecast to be burned for the next day.

2.5. Initial and Boundary Conditions

In AIRPACT-3, initial conditions for each forecast period are from the results of last simulation hour of the previous day’s forecast. This model restart approach maintains the continuity of chemical conditions between periods and reduces the need for model spin-up associated with static initial conditions.

The chemical boundary conditions in AIRPACT-3 are compiled from the MOZART-2 (Ozone and Related Chemical Tracers version 2) [Horowitz et al., 2003] global chemical model to account for seasonal variability of ozone and other chemical species throughout the year [Weiss-Penzias et al., 2004]. Long-term MOZART-2 simulation results (1990–1999) were diurnally averaged by month and grid across the forecast domain. The resulting boundary conditions are diurnal concentrations of species that change by month and location. Recent model studies have investigated the effects of using global model output as boundary conditions for regional air quality modeling and showed improvements to model performances [Barna and Knipping, 2006; Tong and Mauzerall, 2006]. Since AIRPACT-3 operates throughout the year, results from global chemistry model provide the most complete and relevant information, and reflect the seasonality of pollutants and pollutant precursors into the forecast domain. For the month of August and September the ozone boundary conditions from

<table>
<thead>
<tr>
<th>Surface Temperature, °C</th>
<th>Wind Direction, deg</th>
<th>Wind Speed, m s$^{-1}$</th>
<th>24-h Precipitation, mm</th>
<th>Relative Humidity, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>MB</td>
<td>−0.3 to 0.6</td>
<td>5 to 8</td>
<td>1.4 to 1.9</td>
<td>−0.8 to 0</td>
</tr>
<tr>
<td>ME</td>
<td>2.1 to 2.4</td>
<td>62 to 70</td>
<td>2.2 to 2.5</td>
<td>1.7 to 2.8</td>
</tr>
</tbody>
</table>
MOZART-2 is similar to those defined in the CMAQ default profile with surface level mixing ratio at 30 to 35 ppbv. The ozone boundary condition starts to differ near the tropopause with MOZART-2 having higher levels than the default CMAQ profile.

2.6. Web Presentation of Results

Following each forecast, input and output data are processed for display on the AIRPACT-3 website (http://www.lar.wsu.edu/airpact-3). Animated maps of meteorological variables, emission rates, and species concentrations are displayed for selected parameters. On the day following the forecast, observations from a regional real-time observational network are automatically retrieved and paired with the model predictions. The observational data are graphed on the model contour maps for web retrieval as historical simulations. The model output is also used to compile monthly maps that include monthly maxima and other accumulated air quality parameters. Finally, the paired observed and predicted concentrations are archived for further analysis and model evaluation.

3. Description of the AIRPACT-3 Evaluation

A comprehensive forecast evaluation was carried out by rerunning the AIRPACT-3 system for August–November 2004 period in forecast mode without observational data. This period was chosen to coincide with a measurement program in the Columbia River Gorge conducted by the Southwest Clean Air Agency. Since this is a historical rerun, the system was initialized with 1-month model spin-up over July 2004. All other model parameters and data input were identical to the forecast system described earlier.

Forecast MM5 meteorological results were compared with measurement data for stations across the domain to assess model performance in terms of the performance statistics defined in Table 2. Table 3 summarizes the performance statistics for variables important to air quality. Overall, MM5 was reasonably accurate for surface temperature, 24-h precipitation and relative humidity, but it slightly over-estimated wind speed. The model statistics show that there can be significant forecast errors in wind direction with mean errors between 62° to 70°. The mean errors in wind speed were approximately 2 m s⁻¹, and for surface temperature the mean error was approximately 2°C. This level of model performance is commonly observed for MM5 forecast simulations for the region, and the performance statistics are generally comparable, but slightly higher than those obtained using MM5 with observational nudged simulations for the same region [Barna and Lamb, 2000; O’Neill and Lamb, 2005].

Wild and prescribed fire emissions were obtained from the BlueSky system with reported fire events during the evaluation period. The monthly fire emission totals for the domain are summarized in Table 1. August 2004 had the highest wildfire activity with all fire emissions contributed from wildfires. The major wildfire events in August were the Porter fire in the Salmon-Challis National Forest near Central Idaho, the French fire in northern California, and the Fischer fire in south central Washington. For other months, fire emissions were dominated by prescribed fires in Washington, Oregon, Idaho and Montana. Wildfire contributes to less than 2% of total fire emissions in these months.

Ozone and PM₂.₅ measurement data for the AIRPACT-3 evaluation were collected from measurement networks for stations in Washington, Oregon and Idaho. Ozone measurements were obtained for 30 stations in the EPA-AQS measurement network (available at http://www.epa.gov/ttn/airs/airsaqs). Total mass PM₂.₅ measurements were obtained for 18 stations in the IMPROVE measurement network (available at http://vista.cira.colostate.edu/improve), and 36 stations in the EPA-AQS network. Several stations also reported chemically speciated fine PM component measurements and were used in the evaluation. Hourly PM component measurements were also obtained from 3 stations in the Columbia River Gorge in the SWCAA measurement program [Green et al., 2006]. The fine PM components

Table 4. Summary of AIRPACT-3 Forecast Performance Statistics for Daily Maximum 8-h Ozone for August–September 2004

<table>
<thead>
<tr>
<th></th>
<th>N</th>
<th>MB, ppbv</th>
<th>ME, ppbv</th>
<th>NMB</th>
<th>NME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Predicted mean, ppbv</td>
<td>46</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Measured mean, ppbv</td>
<td>43</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 2. Ratio of predicted to measured daily maximum 8-h ozone versus the measured values during August–September 2004.
include particulate nitrate (PNO3), sulfate (PSO4), ammonium (PNH4), elemental carbon (PEC) and organic carbon (POC). Figure 1 depicts the location of these observation stations within the domain. The IMPROVE stations were mostly in Class I wilderness areas and national parks. The EPA-AQS stations were mostly in urban and suburban areas. The measurement program by the SWCAA was limited to within the Columbia River Gorge.

4. Evaluation Results and Discussion

4.1. Ground Level Ozone Forecast

[25] Forecast ozone mixing ratio from AIRPACT-3 were extracted from grid cells representing measurement location and paired by site and time for comparisons. Hourly ozone forecast and measurement data were processed to yield daily maximum 8-h averaged (DM8H) values over the August–September 2004 period for the evaluation.

[26] During the 2 month period, there were no measured ozone exceeding the 80 ppbv NAAQS standard, however, ozone levels greater than 70 ppbv were observed. The mean measured DM8H ozone over all sites was 43 ppbv, and highest observed value was 79 ppbv at North Bend, WA downwind of Seattle. In comparison, the mean forecast DM8H ozone over all sites was 46 ppbv, and highest forecast value was 87 ppbv at Enumclaw, WA, also downwind of Seattle. Both forecast and observed peak DM8H occurred on 10 August. The AIRPACT-3 system captured the temporal peak ozone onset and the general pollutant conditions during the 2 months with 95% of all predicted
values within a factor of two of the corresponding measured values.

The overall DM8H ozone forecast performance statistics are summarized in Table 4. These standard model performance statistics are defined in Table 2 and are used in many recent air quality model evaluation studies [Bailey et al., 2007; Eder and Yu, 2006; Hogrefe et al., 2007; Tong and Mauzerall, 2006; Zhang et al., 2006]. Data with measured ozone mixing-ratio less than 30 ppbv were excluded to emphasize high ozone events important for air quality forecasts. Overall, AIRPACT-3 slightly over-predicted DM8H ozone with a mean bias (MB) of 2.7 ppbv and normalized mean bias (NMB) of 6%. The mean error (ME) was 7.2 ppbv and normalized mean error was (NME) 17%. This model performance is reasonable compared to the range of statistics in other CMAQ evaluation studies for the same region [Smyth et al., 2006; O’Neill et al., 2006b].

Given that all model inputs are forecast conditions without observational analysis, the AIRPACT-3 system is fairly accurate in predicting the daily peak ozone levels for the region.

A more quantitative comparison in Figure 2 shows the ratio of predicted to measured DM8H ozone versus the corresponding measured values for August and September. Data were compiled from all 30 ozone stations. A ratio of one indicates perfect forecast agreement. AIRPACT-3 performed better at predicting high ozone conditions above 50 ppbv, but systematically over-predicted observed levels less than 40 ppbv. The over-prediction was worse with lower observed ozone. This systematic over-prediction during low ozone conditions is frequently observed [Russell and Dennis, 2000], and can be caused by a combination of several factors. In a CMAQ evaluation study for the eastern U.S., Eder et al. [2006] attributed the over-prediction to excessive downward transport of high level ozone aloft and too much photolysis under high cloud conditions. The positive ozone bias has also been linked to poor representation of the mixed layer in coastal regions, [Gilliam et al., 2005; Zhang et al., 2006] as well as higher ozone chemical production rate with the SAPRC99 chemical mechanism used in the AIRPACT-3 system [Arnold and Dennis, 2006]. For some periods, the boundary conditions from the global model could also contribute to overestimation of low levels of surface ozone.

### 4.1.1. Spatial Ozone Forecast

The August and September averaged DM8H ozone from AIRPACT-3 forecast and measurement stations are presented in Figure 3. The ozone spatial distribution varied between the 2 months, with August having generally higher ozone than September. The modeled and observed data for both months showed higher ozone levels in the inland areas than along the coastal regions.

In August, ozone levels of 40 ppbv to 48 ppbv for sites west of the Cascade Mountain were captured by the model while slightly higher levels of 45 ppbv to 54 ppbv were reasonably forecast for sites east of the Cascade Mountain and in Idaho. Ozone mixing ratios for sites within Seattle and Portland urban areas were slightly over-predicted. In Boise, ID, the peak ozone occurred in August with an observed average DM8H ozone of 54 ppbv; AIRPACT-3 system predicted close to this with 51 ppbv.

In September, ozone levels were lower, and AIRPACT-3 over-predicted some of the measurements along the coastal regions of the domain. Ozone between 30 ppbv to 42 ppbv for Seattle and Portland urban areas were over-predicted possibly due to combinations of boundary condition influence and poor model representation of the mix layer along the coast. AIRPACT-3 correctly captured the higher levels east of the domain. Peak ozone during the month occurred at the Craters of the Moon site (+43.461N, −113.562W) in Idaho with observed DM8H ozone of 45 ppbv; AIRPACT-3 predicted 50 ppbv.

Performance evaluation by site over the 2-month period showed forecast DM8H ozone are generally positively biased due to over-predictions of low observed ozone levels. The NMB values ranged from −3% at Talent, OR (+42.229N, −122.788W) to 21% at the Olympic National Park, WA, (+48.098N, −123.426W), and of the total 30 measurement sites, 17 sites had NMB within ±10%. The NME site statistic ranged from 10% at Marblemount, WA (+48.539N, −121.447W) to 23% at Mt. Rainier National Park, WA, (+46.785N, −121.733W) and of the total 30 stations, 22 sites had NME less than 20%.

Comparisons between 13 urban/suburban and 17 rural measurement locations showed slightly better perfor-
mance statistics for urban/suburban sites with the average NMB of 5% and the NME of 16%. The observed mean DM8H ozone was 70 ppbv and AIRPACT-3 predicted 74 ppbv. AIRPACT-3 had better skill in capturing high ozone conditions, but over-predicted the lower, rural ozone. At rural sites, the mean observed DM8H ozone was 59 ppbv and AIRPACT-3 over predicted at 66 ppbv. The performance statistics were also slightly worse with NMB of 10% and NME of 17%.

Figure 5. Predicted (dotted line) and measured (solid line) average diurnal hourly ozone for the 7–17 August 2004 period. Measurements are from sites in the EPA-AQS network. The top and bottom error bars represent 75th and 25th percentile values and the center solid line indicates the mean.
4.1.2. Temporal Ozone Forecast

[34] Ozone forecast by AIRPACT-3 tracked closely with the measurements averaged across all sites during August–September 2004. Figure 4 shows the time series of averaged DM8H ozone and the corresponding model statistics (ME, MB). The overall correlation coefficient between observed and predicted DM8H ozone concentrations (r) is 0.58. Maximum site averaged measured DM8H ozone occurred on 12 August with 58 ppbv. AIRPACT-3 correctly predicted the temporal pollution onset, but over-predicted the magnitude with 63 ppbv. During the week of elevated ozone, AIRPACT-3 was able to capture the trend of elevated ozone pollution with a bias between −5 and 5 ppbv. The system predicted the pollution episode to end 3 d earlier than observed. After 20 August when averaged observed MD8H ozone were relatively low, AIRPACT-3 over-predicted ozone with generally positive mean bias and mean error between 0 and 15 ppbv.

[35] The elevated DM8H ozone during 7–17 August was due to a high pressure system over the region causing light winds and high temperatures. Elevated ozone conditions were observed downwind of most urban centers. Figure 5 shows the averaged diurnal hourly ozone concentrations for 10 EPA-AQS measurement sites during this period. These sites were selected to show model performance for locations with high ozone. Comparisons between the predicted and measured hourly ozone demonstrate the system’s ability to capture the pollution variability at these sites. The magnitude of daytime ozone maxima in the afternoon were reasonably captured at most sites. The largest difference between predicted and observed averaged ozone maxima was at Carus, OR, where AIRPACT-3 predicted 68 ppbv and the observed average was 56 ppbv. There were a few under-predictions of the daily peak concentrations, but the magnitude differences were very small. The worse under-prediction was at Lake Sammamish, WA; AIRPACT-3 under-predicted the average ozone maxima by 4 ppbv. AIRPRACT-3 also predicted the ozone diurnal pattern very well. The system captured the rise and fall of ozone variations, and the timing of daily peak was predicted to within two hours of the measured occurrence. However, it is also clear that the system performed poorly at night. It over-estimated the mean nighttime low ozone at most locations. At many urban sites, the predicted nighttime ozone never got below 20 ppbv when the measured ozone levels were near zero. Some recent studies suggest this poor nighttime model performance is due to incorrect model representation of the nocturnal boundary layer. The errors in vertical mixing may dilute NO emissions at night and suppress the chemical removal of ozone (O₃ + NO → O₂ + NO₂) [Eder et al., 2006; Zhang et al., 2006].

[36] Over the August–September 2004 evaluation period, AIRPACT-3 was able to capture the overall hourly onset of daily ozone maxima. Figure 6 shows the distribution of hourly differences between the predicted daily peak occurrence time and the observed ozone peak time. Of the 1823 observed and modeled paired data points, 20% of the time the model was accurate within the hour in predicting the daily peak ozone occurrence, and 75% of the time the model was accurate to within 3 h of the observed ozone maxima.

4.2. Surface PM₂.₅ Mass Concentration Forecast

[37] Predicting PM concentrations is considerably more difficult than for gas-phase pollutants [Seigneur, 2001]. Simulating PM formation involves tracking the transport and interactions of both primary and secondary pollutants across gas, solid and aqueous phases. Furthermore, measurements of particulate matter are less abundant and contain higher uncertainties. Since measurement methods, uncertainties and errors associated with monitor networks differ, the evaluation of the PM forecast is separated by measurement networks. This also provides a general performance comparison between urban and rural regions as most EPA-AQS network sites are in urban areas while the IMPROVE sites and the SWCAA sites are in rural locations. PM measurements were based on mass concentration averaged over a 24-h period. The hourly AIRPACT-3 forecasts were averaged over the same period for comparison.

[38] Table 5 summarizes the PM₂.₅ performance statistics by measurement network. The IMPROVE network monitors at rural locations had lower mean observed concentration of 6.8 µg m⁻³ compared to the urban EPA-AQS network sites of 11 µg m⁻³. AIRPACT-3 captured this overall difference, albeit with slight over-prediction. The average predicted PM₂.₅ concentrations were 9 µg m⁻³ and 13 µg m⁻³.

Table 5. Summary of AIRPACT-3 Forecast Performance Statistics for 24-h PM₂.₅ by the EPA-AQS and IMPROVE Measurement Networks for August–November 2004

<table>
<thead>
<tr>
<th></th>
<th>EPA-AQS</th>
<th>Improve</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>1014</td>
<td>234</td>
</tr>
<tr>
<td>MB, µg m⁻³</td>
<td>2.1</td>
<td>2.2</td>
</tr>
<tr>
<td>ME, µg m⁻³</td>
<td>8.0</td>
<td>5.5</td>
</tr>
<tr>
<td>NMB</td>
<td>17%</td>
<td>32%</td>
</tr>
<tr>
<td>NME</td>
<td>70%</td>
<td>81%</td>
</tr>
<tr>
<td>FB</td>
<td>3%</td>
<td>2%</td>
</tr>
<tr>
<td>FE</td>
<td>59%</td>
<td>54%</td>
</tr>
<tr>
<td>Predicted mean, µg m⁻³</td>
<td>13</td>
<td>9.0</td>
</tr>
<tr>
<td>Measured mean, µg m⁻³</td>
<td>11</td>
<td>6.8</td>
</tr>
</tbody>
</table>
Figure 7. Fractional bias (top) and fractional error (bottom) of AIRPACT-3 PM$_{2.5}$ predictions against measured concentrations for EPA-AQS (cross) and IMPROVE (dot) sites. Model performance goal and criteria ranges are represented by dotted and solid lines, respectively.

respectively. Of all the forecast comparisons, 61% fall within a factor of 2 of measurement values, and in contrast to the ozone forecast performance, there was no clear concentration range where AIRPACT-3 performed better.

[39] Additional performance measures specifically for PM are fractional bias (FB) and fractional error (FE) as recommended by Boylan and Russell [2006] who suggested performance goals and criteria for these two statistics. These statistics allow for less stringent criteria at low concentrations to account for higher uncertainties near detection limits. In this evaluation, AIRPACT-3 achieved an overall FB of 3% and FE of 58%. The FB was within the recommended model performance goal of ±30%. The FE exceeded the goal, but was bordering the performance criteria limit of 60%. Figure 7 shows the monthly FE and FB site statistics against their monthly measured concentrations. Between the EPA-AQS and IMPROVE network monitors, PM$_{2.5}$ concentrations at the EPA-AQS sites are higher and exhibit more scatter due to urban influences. Most sites had monthly PM$_{2.5}$ concentrations between 7 µg m$^{-3}$ and 15 µg m$^{-3}$. A few sites had monthly PM$_{2.5}$ concentrations near 30 µg m$^{-3}$. Overall, AIRPACT-3 performed well in predicting the measured concentrations with most points within the model performance criteria limit. Among all the comparisons, IMPROVE sites had 82% and 77% of data points within the criteria limit for FE and FB, while the EPA-AQS sites had, 68% and 61% within the criteria limit.
4.2.1. Spatial PM$_{2.5}$ Forecast

[40] The spatial distribution of PM$_{2.5}$ concentrations varied significantly due to occurrences of wildfires and anthropogenic pollution from urban areas. Figure 8 compares the AIRPACT-3 predicted PM$_{2.5}$ concentrations and the corresponding measurement concentrations for August and November. August had the highest predicted domainwide concentrations because of numerous wildfires occurrences. The Porter Fire in central Idaho was the largest fire event in the region, and it burned throughout August. It resulted in large regional impacts with very high PM$_{2.5}$ concentrations. Pollution impacts from smaller fires in central Washington, southern Oregon and southern British Columbia were also predicted with hot spots of elevated PM$_{2.5}$ concentrations exceeding 35 $\mu$g m$^{-3}$.

[41] Wildfire activity decreased for the rest of the months, and the predicted monthly PM$_{2.5}$ spatial distributions were more similar to November, with elevated concentrations in urban areas: Seattle, Portland, Spokane, Boise, and along major highways.

[42] AIRPACT-3’s forecast performance varied by sites and months. It performed slightly better for sites along the Interstate-5 highway (I-5) corridor in the western part of the domain compared to sites east of the Cascades. PM$_{2.5}$ concentrations south of Seattle and Portland urban areas were reasonably predicted. August had the worst overall

Figure 8. Monthly averaged PM$_{2.5}$ predicted concentration contours ($\mu$g m$^{-3}$) and the corresponding measured concentrations (underline) for August and November 2004.
PM$_{2.5}$ forecast compared to the rest of the months. The system significantly over-predicted PM$_{2.5}$ concentrations in Idaho. In August, 47% of all sites exceeded the model criteria limit for FB and, 30% exceeded that for FE. AIRPACT-3 performed better for the other months with more than 75% of all sites within the criteria limit for both FE and FB.

The poor PM$_{2.5}$ forecast performance in August can be attributed to over-predictions for sites downwind of fire events. This error is partly due to uncertainties in wildfire emission estimates and the modeling error in fire plume transport. Since fire emissions are modeled as point sources rather than area sources, their emissions are confined in one or two grid points in the model domain at each source locations. This can result in high positive biases in forecast PM$_{2.5}$ for sites near the emission sources as observed in the evaluation. Errors in MM5 wind direction and wind speed can also lead to incorrect shifts in fire plume centerline resulting in significant biases between predicted and observed concentrations. For example, the August observed PM$_{2.5}$ at Boise, ID (+43.562N, -116.563W) was 5 $\mu g$ m$^{-3}$ and AIRPACT-3 overestimated this with 16 $\mu g$ m$^{-3}$.

### 4.2.2. Temporal PM$_{2.5}$ Forecast

Figure 9 shows the August–November time series of predicted and measured daily PM$_{2.5}$ concentrations, and the corresponding performance statistics (FE, FB) averaged across the EPA-AQS measurement sites (top) and the IMPROVE measurement sites (bottom).

<table>
<thead>
<tr>
<th>Day</th>
<th>Predicted</th>
<th>Measured</th>
<th>FB</th>
<th>FE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aug/1</td>
<td>20</td>
<td>10</td>
<td>-10</td>
<td>30</td>
</tr>
<tr>
<td>Aug/10</td>
<td>25</td>
<td>15</td>
<td>-5</td>
<td>40</td>
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<td>Aug/19</td>
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<td>20</td>
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<tr>
<td>Aug/28</td>
<td>35</td>
<td>25</td>
<td>15</td>
<td>60</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Day</th>
<th>Predicted</th>
<th>Measured</th>
<th>FB</th>
<th>FE</th>
</tr>
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<tbody>
<tr>
<td>Sep/6</td>
<td>30</td>
<td>20</td>
<td>10</td>
<td>40</td>
</tr>
<tr>
<td>Sep/15</td>
<td>35</td>
<td>25</td>
<td>15</td>
<td>50</td>
</tr>
<tr>
<td>Sep/24</td>
<td>40</td>
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<td>20</td>
<td>60</td>
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<td>Oct/3</td>
<td>45</td>
<td>35</td>
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<td>Oct/30</td>
<td>60</td>
<td>50</td>
<td>40</td>
<td>100</td>
</tr>
</tbody>
</table>

The concentration range was smaller at the IMPROVE stations, with observed concentrations from 2.7 $\mu g$ m$^{-3}$ to 8.5 $\mu g$ m$^{-3}$, and modeled concentrations from 3.5 $\mu g$ m$^{-3}$ to 18 $\mu g$ m$^{-3}$. The correlation coefficient for the concentration time series is 0.77. The concentration range was larger at the EPA-AQS stations, with observed concentrations from 2.5 $\mu g$ m$^{-3}$ to 28 $\mu g$ m$^{-3}$, and modeled concentrations from 4.3 $\mu g$ m$^{-3}$ to 24 $\mu g$ m$^{-3}$. The correlation coefficient is worse at 0.36. The larger concentration range at the EPA-AQS stations resulted in FE
of 8% to 137% compared with the IMPROVE stations of 13% to 96%.

Large concentration fluctuations were observed for the IMPROVE stations in August when wildfire activities were high. During this period AIRPACT-3 over-predicted the fire impacts with FB reaching 68%. For October and November, PM$_{2.5}$ concentrations stayed low and the FB ranged from −24% to 41%. At the urban sites, represented by the EPA-AQS stations, large concentration fluctuations were observed during October and November when stagnant atmospheric conditions were more frequent. During these 2 months AIRPACT-3 performed fairly well. The system over-predicted the elevated concentrations in early October with FB ranging 4% to 74% and slightly under predicted the period peak concentration in early November with FB ranging from 0% to −33%.

4.3. Speciated PM$_{2.5}$ Component Forecast

CMAQ simulates the transport and chemistry of individual inorganic and organic aerosol species to produce total PM$_{2.5}$ mass concentration. The accuracy of the PM$_{2.5}$ forecast, thus, depends on the correct representation of speciated aerosol composition. Measurement data for aerosol components were available from 18 IMPROVE sites, eight EPA-AQS sites and three SWCAA sites. Since the IMPROVE and EPA-AQS measurements were 24-h averaged values, the hourly measurements from the SWCAA sites were converted to the same time averaged basis for comparisons. Figure 10 shows averaged monthly aerosol component concentrations from AIRPACT-3 and the corresponding measurement values by monitor networks. Table 6 summarizes the model performance statistics for individual aerosol species. AIRPACT-3 performed well in predicting the aerosol composition differences for the IMPROVE and EPA-AQS sites, but underestimated several major PM species in the Columbia River Gorge, represented by the SWCAA sites. The forecast accuracy varies by month and observation networks. Overall, AIRPACT-3 over-predicted PEC, and significantly underestimated PSO$_4$. Forecast performance was better for PNH$_4$ and PNO$_3$ for stations in the EPA-AQS and IMPROVE measurement networks.

The system correctly predicted POC as the major aerosol component for all months and measurement networks. The average observed POC concentrations were 5.2 μg m$^{-3}$, 2.3 μg m$^{-3}$, and 2.5 μg m$^{-3}$ for EPA-AQS, IMPROVE and SWCAA sites, respectively; AIRPACT-3 simulated this with 5.5 μg m$^{-3}$, 1.9 μg m$^{-3}$ and 2.3 μg
m\(^{-3}\). Additional analysis showed large over-predictions of POC above 8 \(\mu g\) m\(^{-3}\). The over-predictions occurred mostly in August during high wildfire activity. Since 77% of all PM\(_{2.5}\) from fire are allocated to primary organic aerosol (POA), errors in fire emission estimates or fire plume transport can cause POC to dominate the PM\(_{2.5}\) fraction. Moreover, POC is difficult to model due to uncertainties in POA and VOC emission inventories and the complex chemistry involved in secondary organic aerosol formations.  

[48] PEC represents 16% of total primary fire PM\(_{2.5}\) and is the second major aerosol component in emissions. AIRPACT-3 over-predicted PEC in all three measurement networks. The MB are 0.5 \(\mu g\) m\(^{-3}\), 0.4 \(\mu g\) m\(^{-3}\) and 0.2 \(\mu g\) m\(^{-3}\) respectively for the EPA-AQS, IMPROVE and SWCAA sites. Similar to POC, AIRPACT-3 tends to systematically over-predict PEC for observed concentrations above 1 \(\mu g\) m\(^{-3}\).  

[49] PSO\(_4\) is the second major aerosol components in all three measurement networks, AIRPACT-3 significantly under-predicted PM\(_{2.5}\) from this fraction. The negative bias is largest in the Columbia River Gorge with MB of \(-1.9\) \(\mu g\) m\(^{-3}\). The performance of PSO\(_4\) is considered to be poor compare with other model studies using CMAQ for the region [O’Neill et al., 2006a; Smyth et al., 2006]. Model performance for PSO\(_4\) was expected to be better given that the CMAQ sulfate science algorithms were developed earlier in the Regional Acid Deposition Model [Stockwell et al., 1990] and are comparatively better understood than the organic aerosol components. PSO\(_4\) comes from oxidation of gas-phase SO\(_2\) and the direct emission of sulfate particles. The results suggest probable under estimation of SO\(_2\) and/ or primary sulfate emissions.  

[50] PNO\(_3\) was slightly under-predicted for all months and all sites, except October. The measured concentrations at the EPA-AQS, IMPROVE and SWCAA sites were 1.2 \(\mu g\) m\(^{-3}\), 0.8 \(\mu g\) m\(^{-3}\) and 0.8 \(\mu g\) m\(^{-3}\) respectively; AIRPACT-3 under-estimated the average with 0.9 \(\mu g\) m\(^{-3}\), 0.6 \(\mu g\) m\(^{-3}\) and 0.3 \(\mu g\) m\(^{-3}\). Despite the under-predictions, model performance for PNO\(_3\) is considered to be good when compared with other air quality model studies in the literature [Eder and Yu, 2006; Makar et al., 2003; O’Neill et al., 2006b; Smyth et al., 2006]. The good performance in this evaluation may reflect better representation of regional NH\(_3\) and NO\(_x\) emissions, and the updated science algorithms in the current inorganic aerosol module.  

[51] Observations for PNH\(_4\) were only available for the EPA-AQS sites and two stations (COGO, CORI) in the SWCAA network. The COGO site (+45.569N, −122.210W) and the CORI sites (+45.664N, −121.001W) were 20 km and 100 km east of Portland, OR, respectively. In this evaluation, AIRPACT-3 slightly under-predicted PNH\(_4\) in both networks with ME of 0.4 \(\mu g\) m\(^{-3}\). This overall model performance of PNH\(_4\) is considered to be good for the region when compared with other model studies [O’Neill et al., 2006b; Smyth et al., 2006]. PNH\(_4\) has been very difficult to model correctly due to high uncertainties in regional ammonia emission estimates and complex chemical interactions [Park et al., 2006].  

[52] Predictions in the Columbia River Gorge, represented by the SWCAA sites, were slightly poorer with mostly under-prediction, particularly for PSO\(_4\). The poor model performance was not surprising due to the complexity of terrain within the Gorge. The model resolution of 12-km is insufficient to properly resolve the complex transport of pollutants and their precursors within the Gorge topography.

[53] A separate comparison in Figure 11 shows the hourly predicted and measured PM\(_{2.5}\) component concentration comparisons for the SWCAA sites. Overall, AIRPACT-3 was able to capture the general temporal concentration trends; but it failed to duplicate the fine pattern of hourly concentrations. Modeling aerosol concentration variations at short temporal timescales is more difficult due to large concentration gradients, and higher uncertainties in estimating PM, and PM precursor gas emissions [Seigneur, 2001]. The significant under-prediction of PSO\(_4\) is clearly evident.
with predicted concentrations less than $2 \, \mu g \, m^{-3}$ and measured values ranging from $1 \, \mu g \, m^{-3}$ to $10 \, \mu g \, m^{-3}$. The forecast was slightly better for PNO3. However, similar to PSO4, the system failed to simulate the episodic conditions observed in the Gorge in early November. There were occasional spikes of high predicted POC and PEC concentrations throughout the period. These were likely due to shifting of fire emission plumes impacting the monitor sites.

### 4.4. November Stagnant Period

A stagnant atmospheric condition was observed for a two-week period beginning 3 November when low ventilation trapped pollutants near surface and resulted in elevated PM$_{2.5}$ concentrations exceeding the EPA NAAQS. Elevated concentrations were predicted along the west coast, in eastern Washington and in the Idaho Treasure Valley. Monitor sites in Seattle, WA (+47.563N, -122.338W); Portland OR (+45.561N, -122.679W); and Boise, ID (+43.562N, -116.563W) had high observed concentrations.

**Figure 12** shows the time series of predicted and measured daily PM$_{2.5}$ concentrations for the three locations. In Seattle and Portland, the observed PM$_{2.5}$ concentrations were high for the first three measurement periods, and decreased slightly at the end of the event. In Boise, the concentrations were generally lower, but peaked on 8 November when PM$_{2.5}$ reached $44 \, \mu g \, m^{-3}$. AIRPACT-3 captured the overall concentration trends, but overpredicted at Seattle and Portland. Predictions were better at the Boise site, but AIRPACT-3 missed the period maximum with a modeled PM$_{2.5}$ concentration of $36 \, \mu g \, m^{-3}$.

**Figure 13** shows the predicted and measured aerosol component concentrations and their percentage fraction with respect to the total PM$_{2.5}$ at the three urban sites. A closer look showed that even though the total PM$_{2.5}$ was well predicted at Boise, the component concentrations were
inaccurately represented. AIRPACT-3 under predicted all aerosol components at Boise, especially the dominate PNO3 and POC. Comparing the percentage fraction at Boise, the speciated PM components represented much higher total PM$_{2.5}$ than predicted in AIRPACT-3. The major predicted component in Boise was unspecified other PM$_{2.5}$. This suggests that the model under-predicted PM$_{2.5}$ contributions from secondary speciated PM components, and overpredicted contributions from primary emission such as fine soil for this period.

PM components at Seattle and Portland were better predicted. AIRPACT-3 correctly predicted the dominant POC component, and concentrations of PNH4 and PNO3 during this period. The total PM$_{2.5}$ concentration fractions were better captured, however, the model still underrepresented the total PM$_{2.5}$ contributions from the speciated aerosol species.

### 5. Impacts of Fire and Dairy Ammonia Emissions on PM$_{2.5}$ Forecast

Two emission sensitivity simulations were conducted to quantify the impacts of the fire and dairy ammonia emissions to PM$_{2.5}$ forecast performances in AIRPACT-3. The simulations were performed with the same AIRPACT-3 framework described earlier, but emissions input were modified by withholding fire emissions (noWF case) or the dairy ammonia emissions (noNH3 case) separately, while keeping all other emissions unchanged. The impacts on the AIRPACT-3 forecasts were analyzed by comparing the predicted PM$_{2.5}$ concentrations from the two cases with measurements and with the original AIRPACT-3 results (base-case).

The fire emissions sensitivity was analyzed for August 2004 when fire occurrence was the highest. The period averaged 24-h PM$_{2.5}$ for the IMPROVE and the EPA-AQS measurement networks were 6 μg m$^{-3}$ and 7 μg m$^{-3}$, respectively. In the base-case, AIRPACT-3 predicted 4 μg m$^{-3}$ and 5 μg m$^{-3}$. In the noWF case, the reduced fire PM emissions resulted in even lower PM$_{2.5}$ concentrations at 2 μg m$^{-3}$ and 4 μg m$^{-3}$, respectively. Removing fire emissions from the AIRPACT-3 system degraded the overall PM$_{2.5}$ forecast with higher negative biases. The changes are slightly larger for the rural sites, represented by the IMPROVE network monitors. Without fire emissions, the forecast performance for rural sites in terms of FB and FE are −91% and 96%. This is slightly worse compared to the base-case where FB is −68% and FE is 93%. Changes at specific measurement sites were greater in Idaho and Washington where the wild fire events produced significant amounts of PM emissions. Figure 14 shows the average 24-h PM$_{2.5}$ concentration time series in the area for the two cases together with measured values at the EPA-AQS and IMPROVE networks. Measured concentrations peaked in the middle of the month, and AIRPACT-3 with fire emissions was able to predict the overall concentration changes. When compared with PM$_{2.5}$ concentrations without fire emissions, the system consistently under-predicted PM$_{2.5}$ impacts for both urban and rural locations.

Spatially the PM$_{2.5}$ concentration distribution for the noWF case changed significantly compared to the base-case. The PM$_{2.5}$ concentration hot spots in Figure 8 as result of wild fires disappeared, and the concentration distribution
on the overall PM<sub>2.5</sub> concentrations in the area and, in turn, there was little change to AIRPACT-3 forecast performance. For the 2-week period, the average measured 24-h PM<sub>2.5</sub> in IMPROVE and EPA-AQS networks were 5 µg m<sup>-3</sup> and 21 µg m<sup>-3</sup>, respectively. AIRPACT-3 predicted 6 µg m<sup>-3</sup> and 22 µg m<sup>-3</sup> in the base-case, and in the noNH3 case, the total PM<sub>2.5</sub> decreased only by 0.5 µg m<sup>-3</sup> and 1.5 µg m<sup>-3</sup>, respectively, when compared to the base-case. The overall model performance statistics for PNO3, PSO4 and PNH4 changed minimally. This is not surprising since ammonia emissions from dairy only accounts for only 6% of total ammonia emissions in the region, and the sources are more isolated and not well represented by the measurement sites. In addition, changing ammonia gas in CMAQ influenced PM<sub>2.5</sub> formation only through inorganic nitrates and sulfates which represent very small mass fractions of the total PM<sub>2.5</sub> in the base-case.

A closer look at PM<sub>2.5</sub> concentrations at individual sites revealed that removing dairy ammonia emission can influence secondary inorganic chemistry conditions at specific locations thus alter the predicted PM<sub>2.5</sub> concentrations. For example, at Portland OR, one of the EPA-AQS sites, the average measured PM<sub>2.5</sub> concentration for the period was 23 µg m<sup>-3</sup> and AIRPACT-3 overpredicted in the base-case with 47 µg m<sup>-3</sup>. In the noNH3-case, when dairy ammonia emissions were removed, the average predicted PM<sub>2.5</sub> concentration reduced by 3 µg m<sup>-3</sup>. This reduction is from the decreases of not just PNH4 but also PNO3 and PSO4 secondary aerosols. In this case, the component concentrations reduced by 5% to 15% from the base-case. Reducing ammonia in the atmosphere inhibits the formation of ammonium nitrate and ammonium sulfate particles, thus reduces the inorganic aerosol contributions to total PM<sub>2.5</sub>. This, however, has minimal change to AIRPACT-3’s overall PM<sub>2.5</sub> forecast performance because aerosol composition at the site was dominated by POC and PEC components.

6. Summary and Conclusion

We have presented an implementation of a new numerical model framework to an existing regional air quality forecast system, and demonstrated its ability to forecast ground level ozone and PM<sub>2.5</sub> concentrations. The new AIRPACT-3 modeling system uses forecast MM5 meteorology, and the coupled SMOKE emission processor and CMAQ chemical transport model to predict hourly concentrations of air pollutants including ground level ozone and fine particulate matter (PM<sub>2.5</sub>) for the Pacific Northwest region.

The dynamic emission processor explicitly accounts for hourly changes in emissions due to anthropogenic activity patterns and meteorology. By interfacing with the BlueSky system at USDA Forest Service, AIRPACT-3 incorporates realistic fire occurrences for individual fire events in the region. The ammonia emissions module generates hourly emissions by dairy operations and meteorological conditions input to the system.

The forecast system was evaluated for the August–November 2004 period by comparing forecast results with available measurement data from three monitor networks: EPA-AQS, IMPROVE and SWCAA. Results showed the system performed well for both ground level ozone and PM<sub>2.5</sub> predictions.
AIRPACT-3 predicted DM8H ozone levels greater than 70 ppbv during the August–September period. The forecast skills were good with 95% of all data points within a factor of two of the observed concentrations. The system slightly over-predicted with MB and ME of 2.7 ppbv and 7.2 ppbv, respectively. The system was more skillful in predicting episodic ozone conditions above 50 ppbv, but systematically over-predicted ozone less than 40 ppbv. The system was also accurate in capturing the hourly onset of daily peak ozone within 3 h of the measured occurrence.

Predicted PM$_{2.5}$ mass concentrations were evaluated against measurements for rural and urban sites, represented by IMPROVE and EPA-AQS networks, respectively. The system accurately captured the overall concentration differences between the two networks. The averaged observed concentrations for the IMPROVE and EPA-AQS sites were 6.8 $\mu$g m$^{-3}$ and 11 $\mu$g m$^{-3}$, respectively; AIRPACT-3 predicted at 9.0 $\mu$g m$^{-3}$ and 13 $\mu$g m$^{-3}$, respectively.

Predicted fine aerosol component concentrations for PSO$_4$, PNO$_3$, PNH$_4$, POC and PEC were also compared with available measurement data. Over the 4-month period, AIRPACT-3 predicted the PM component distributions relatively well for the EPA-AQS and IMPROVE monitor sites. Both locations had POC as major component species follow by PSO$_4$. AIRPACT-3 slightly over-predicted PEC, and significantly under-predicted PSO$_4$. Forecast performances were worse for sites in the Columbia River Gorge. The system under-predicted concentrations of most aerosol species, particularly the dominant PSO$_4$ aerosol. The errors were most likely due to insufficient spatial resolution and model’s inability to capture the hourly particulate concentration variations.

A separate emission sensitivity study showed AIRPACT-3 was able to adequately simulate the PM pollution impacts from fire events with the real-time wildfire emissions from the Bluesky model. However there was little impact on the overall PM$_{2.5}$ forecast performance with the dairy ammonia emissions module. When fire emissions were removed from the system, AIRPACT-3 performed worse, and the changes were larger for rural regions with higher wild fire activity. Removing dairy ammonia emissions in Washington and Oregon has little impact on the overall PM$_{2.5}$ forecast. This is because dairy ammonia emissions represent a small fraction of the total ammonia emissions in the inventory, and changes to PM$_{2.5}$ were limited to small mass components of inorganic nitrate, ammonia and sulfate.

This evaluation demonstrated AIRPACT-3’s ability to forecast onset of poor air quality conditions using forecast meteorology and emissions. The system represents significant science and capability improvements to the existing AIRPACT-2 system. As with all operational forecasts, continuous evaluation in concert with input data assessments are necessary to further evaluate and improve AIRPACT-3’s performance accuracy.

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