5.6 IMPACT OF THREE DIMENSIONAL DATA ASSIMILATION ON HIGH RESOLUTION WEATHER AND POLLUTION FORECASTING IN THE LOS ANGELES BASIN

Michael D. McAtee[*], Leslie O. Belsma, James F. Drake, Arlene M. Kishi, and Ann L. Mazuk
The Aerospace Corporation, El Segundo, California

1. BACKGROUND

Air quality predictions for the Los Angeles basin pose particular challenges for the weather forecasts that support them. In addition to transport by the regional scale winds, the forecast must accurately capture the sea and land breeze circulation, and the convectively driven upslope circulation in the mountains surrounding the basin, which can inject pollutants into the strong stable layer aloft, where they can travel far, return to the surface, and contribute to air pollution episodes (Liu and Turco, 1995). A high-resolution weather model is a necessary component of air quality modeling in order to adequately represent the small scale phenomena which are significant to air pollution in this region.

The accuracy of predictions from the fine-scale, limited-area models generally used to support air quality applications can depend on several factors. Some of the more important factors include the nature of the weather phenomenon one is attempting to predict, the model's ability to correctly represent physical processes (e.g., boundary layer turbulence, radiation), the quality of boundary conditions employed, and the initial conditions supplied to the model. The quality of the model initial conditions, in turn depends critically on the number, distribution, and quality of atmospheric observations, as well as the methods used to analyze them. Relatively few observations go into an operational forecast in comparison to the number of forecast quantities. Maximizing the use of all available observations, even if these observations are not direct measures of the model variables, is thus very important when initializing a weather model. The work described below focused on improving fine-scale, real-time predictions from the MM5 over the LA basin through the optimal assimilation of space based and local observations. In Section 2 we describe the observational and other sources of initialization data used in the system. A brief description of the 3-Dimensonal Variational Analysis (3DVAR) system used to assimilate the observational data is given in Section 3. This is followed in Section 4 by a description of the mesoscale forecast model configuration and the data assimilation cycle used. In Section 5 we describe the model verification software developed for this system along with some preliminary verification of forecasts made with and without data assimilation. Finally in Section 6 we discuss our plans for completing our data assimilation impact study along with our plans to improve the real-time forecast system.

2. INITIALIZATION DATA

The system assimilates observational data obtained from local sources as well as from the worldwide observational database of the Air Force Weather Agency (AFWA) in Omaha, Nebraska. The AFWA data includes surface and rawinsonde observations; aircraft reports (AIREP); cloud-drift winds from geostationary satellites (SATOB); and precipitable water and surface wind speed over oceans from the Defense Meteorological Satellite Program (DMSP) Special Sensor Microwave/Imager (SSM/I). Additional data are pulled from servers of the surface networks of the South Coast Air Quality Management District of California (SCAQMD) and the Remote Automated Weather Stations (RAWS) of the Bureau of Land Management (BLM), as well as the boundary layer profiler (BLP) network of NOAA's Forecast Systems Laboratory (FSL). Figure 1 gives examples of some of the numerous observations that were assimilated in the inner model domain at 00 UTC on July 10 2003. The examples given are intended to highlight data that are not typically used in meteorological data assimilation for air quality applications.

To make an acceptable forecast over a domain with significant ocean area, MM5 needs the sea surface temperature (SST) field to be specified reasonably well. Daily operational

[*]Corresponding author address: Michael McAtee, AFWA/The Aerospace Corp., 106 Peacekeeper Dr. STE 2N3, Offutt AFB, NE 68113-4039; e-mail: michael.mcatee@aero.org

global Navy SST fields are obtained from AFWA to specify a SST field that does not change during the forecast period.

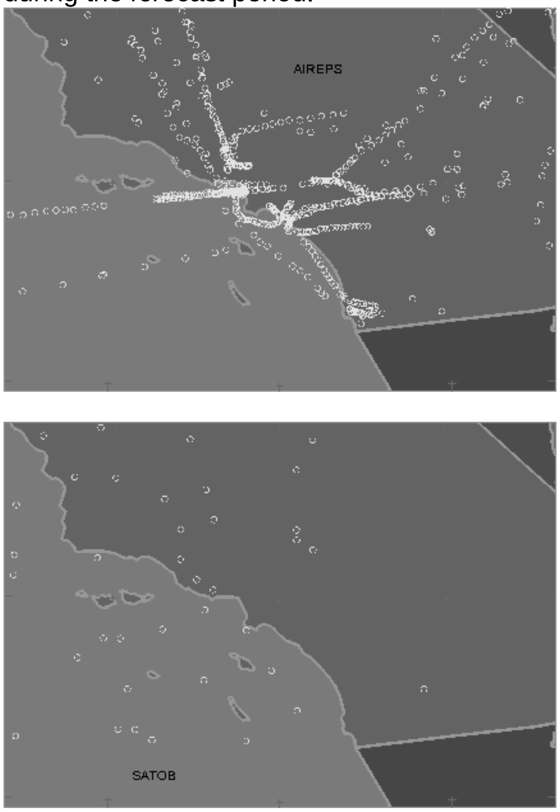


Figure 1. Inner Model Domain AIREP and SATOB Observations for 00 UTC 10 Jul 03

3. THE DATA ASSIMILATION SYSTEM

The 3DVAR system used in this study is fully described by Barker et al (2004) so only a brief description is given below. We chose to use 3DVAR primarily because of its ability to assimilate a wide variety of observations especially those that are not direct measures of the model state variables (e.g., satellite data). 3DVAR categorizes observations by type, each with its own error statistics. Through the laws of physics, (linearized) observation operators relate the values of the model state variables at the analysis time to observed quantities. The goal of three-dimensional assimilation is to specify the model state variables at analysis time so as to minimize the difference between the analysis and observations and a prior estimate of the model state (background). The error statistics of the background field are known extrinsically from prior estimates. In the theory of 3DVAR there is a cost function $J(\mathbf{x})$ given by Equation 1, which is the sum of two terms: one (J^b) depends only on the background field, the other (J^o) depends only on the observations.

$$J(\mathbf{x}) = J^b + J^o = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(\mathbf{y}-\mathbf{y}^o)^T(\mathbf{E}+\mathbf{F})^{-1}(\mathbf{y}-\mathbf{y}^o) \quad (1)$$

where:
$\mathbf{x}$ = a vector of the model variables at a given time (e.g., temperature values on a three-dimensional grid)

$$J^b = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) \quad (2)$$

$$J^o = \frac{1}{2}(\mathbf{y}-\mathbf{y}^o)^T(\mathbf{E}+\mathbf{F})^{-1}(\mathbf{y}-\mathbf{y}^o) \quad (3)$$

$\mathbf{x}^{\boldsymbol{b}}$ = a vector of the model variables at a given time as given by the background field
$\mathbf{B}$ = the matrix of the covariance of error in $\mathbf{x}^{\boldsymbol{b}}$
$\mathbf{y} = \mathbf{Hx}$
$\mathbf{H}$ = the observation operator
$\mathbf{y}^o$= the vector of observations
$\mathbf{E}$ = the (diagonal) matrix of observational (instrumental) error
$\mathbf{F}$ = the "representivity" error matrix, i.e. the error associated with the observation operator
The problem of assimilation reduces to finding the $\mathbf{x}$ that minimizes $J(\mathbf{x})$; the $\mathbf{x}$ that does this is denoted $\mathbf{x}^a$, for analysis. To make it practical to perform the minimization in the time available for analysis, the 3DVAR algorithm uses control variables that are linearly related to $\mathbf{x}$ by a nonsingular transformation rather than directly with $\mathbf{x}$. After J is minimized in the space of control variables, the algorithm inverts the transformation to give $\mathbf{x}^{\mathbf{a}}$.

4. FORECAST MODEL DESCRIPTION

The forecast model used for real-time prediction is version 3.5 of the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model (MM5). MM5 is a limited-area, nonhydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. MM5 has been widely used to support air quality applications and is fully described by Grell et.. al. (1994). The model system is run with two nested domains. Table 1 shows their specifications and Figure 2 shows where they are located. The terrain used is based on a 30 sec (0.9 km) global dataset. In a separate run for each domain, a multiprocessor Cray Research SV1 produces the analyses with a parallel version of 3DVAR. These fields are then used to initialize forecast runs of MM5 on the Cray.

Table 1. Model domain specifications for analysis and forecast

Domain	Grid Box Size (km)	Domain Dimensions (grid boxes)
D01	15	91 x 85
D02	5	121 x 91

Figure 2. Locations of the Model Domains

MM5 is configured as follows: one-way interaction at the boundaries between a parent domain and its child; cumulus parameterization (Grell, 1994) in just the outer domain; cloud radiative cooling; mixed phase ice physics; and a multilayer soil temperature model. Countergradient vertical transport within the planetary boundary layer (PBL) is considered to be significant. The Hong-Pan (1996) scheme, also known as the MRF scheme, is used because it is the only one among the PBL parameterizations offered by MM5 with this feature. MM5 is set to use 37 vertical (half-sigma) levels with the top of the model at 100 hPa.

In order to improve the quality (e.g., fine-scale features) of the background field used by 3DVAR, the near real-time runs of 3DVAR and MM5 are employed in a three-part data assimilation cycle for each domain. Cycle (part) 1 is based at 00 UTC. For this cycle ETA model data at 40 km grid spacing is used as a background field for 3DVAR. The analysis valid at 00 UTC is performed 6-7 hours after valid time to allow for the collection of all possible observations. Atmospheric measurements from satellites often have latencies of a few hours so waiting allows for the use of this data. MM5 is integrated to 6 hours for both domains using 3DVAR's analyses as initial conditions. Cycle 2, which is based at 06 UTC, uses the fine-scale 6-hour forecast for each domain from Cycle 1 as a background field for 3DVAR. Once again the analyses are performed 6-7 hours after 06 UTC to maximize the amount of data used. As in Cycle 1 these analyses are used to initialize MM5 and a 6-hour forecast is produced. Cycle 3, the 12 UTC cycle, is the main forecast cycle. Because of the desire to deliver 24 hours of useful forecast data to air quality forecasters and due to the runtimes of 3DVAR and MM5, Cycle 3 is initiated at 14 UTC. MM5 is integrated out to 36 hours. Graphics for various forecast parameters are created and posted to a web site (http://www.aerospaceweather.com). The digital data in MM5 format is also posted to an ftp site where it is available to personnel from the SCAQMD. Additionally, the daily 36-hour forecasts from Cycle 3 are archived and are available on request. The system has been running routinely since the fall of 2003.

5. MODEL VERIFICATION

Verification software was developed to compare MM5 output to observations. The software interpolates MM5 predictions to the observation location and compares them with measured values, which are taken to be true. The program can compare temperature, relative humidity, dew point, mixing ratio, total precipitable water, wind speed, wind direction. It performs separate comparisons for sounding and surface-station data. For truth data, it reads all the data files from AFWA (surface and rawinsonde observations; AIREPs; GOES cloud-drift winds and DMSP SSMI precipitable water and surface wind speed over oceans), surface station data from RAWS, SCAQMD, and lidar and BLP profiles. Verification scatter plots by forecast hour, with domain biases and RMSE's, are posted to the web site as they become available. Individual times series of model forecasts and corresponding surface observations for a number of SCAQMD sites are also posted.

Because this effort is geared toward supporting air quality forecasting, verification of surface and near surface parameters is of particular importance. The verification efforts are not complete but we began with the verification of surface parameters against the surface measurement network of the SCAQMD. All verification statistics are computed using the hourly output from the 12 UTC (5 AM PDT) based domain 2 (5 km grid-spacing) forecast integrations for the following 21 days: 31 August 2004, 1-11 September 2004, 13-15 September 2004, 24-29 September 2004. The with-local-data-assimilation integrations are based on the operational data assimilation cycle described above while the without-local-data-assimilation runs are initialized with the 06 UTC based ETA model forecasts. The intent is to mimic what most regional real-time model efforts that support air quality applications do. They generally do not employ data assimilation and usually just interpolate the coarser scale model data to their domains. Timely delivery of forecast fields to AQ forecasters generally requires the use of forecast fields from the coarser-scale model for initialization and not analysis fields. It should be noted that the fields used in the without-local-data-assimilation integrations have reaped the benefits of data assimilation as the Eta has its own data assimilation system that utilizes many, though not all, of the same observation sources used in this study. The Eta Data Assimilation System (EDAS) also uses observations that this 3DVAR system does not have the ability to assimilate. Chief among this data are radiance measurements from polar orbiting satellite systems. However the Eta data assimilation is done at a coarser resolution and may not contain the fine-scale detail needed for air quality applications. Figure 3 shows the verification of the 2-meter hourly temperature forecast as a function of forecast hour. The 2-meter temperature is taken directly from the MRF PBL scheme and is not interpolated from the lowest model sigma layer as is typically done. It is clear that the with-data-assimilation run has a superior temperature forecast in the first 2 hours of the forecast. The without data assimilation run has a large warm bias and the RMSE for the with-data-assimilation run is nearly a degree and half lower at the 1-hour point. However the without-data-assimilation run has a slightly lower RMSE at the 3- and 4-hour points despite its poorer performance at the 1 and 2 hour points. The reason for this better forecast at the 3- and 4-hour points would appear to be compensating errors. The MM5 tends to under forecast the maximum temperature and predict it too late in the day. This fact along with the higher, though erroneous, starting temperature of the without-data-assimilation run leads to a slightly more accurate maximum temperature. This point is best illustrated by examination of an individual station's time series of observed temperature versus predicted temperature for the with- and without- data-assimilation cases. The without-local-data-assimilation one-hour prediction for the SCAQMD site at Fontana on 1 September 2004 is nearly 8 degrees too warm. Similarly the two-hour forecast is off by nearly 3 degree. The corresponding forecasts for the with-local data-assimilation are much more accurate. Despite the more accurate prediction in the first two hours the with-data-assimilation maximum temperature forecast is slightly less accurate than the without-data-assimilation case. The with-data-assimilation prediction is again better than the corresponding without data assimilation prediction in the overnight hours though both over forecast temperature. Near the end of the forecast one can see that both predictions are nearly the same. We attribute this to the fact that the lateral boundary conditions for the outer domain are the same for both cases. This eventually drives the prediction in both cases to the same values. This effect might be evident sooner if assimilation was not being done on the outer domain in the with data assimilation case. The verification of 10-meter wind was also accomplished for this period. Wind direction and speed were verified. In terms of wind direction there appears to be no significant difference between the cases at any forecast hour. The wind speed verification shows that the with data assimilation predictions are slightly worse in the first hours of the forecast. We believe this may be due to the geostrophic balance constraint 3DVAR employs. This constraint allows wind information to be inferred from mass information and visa versa. This constraint is lessened or eliminated in areas where it is not appropriate (the PBL and low latitudes) by the use of regression coefficients. These regression coefficients are a part of the background errors statistics. These results suggest a further examination of these statistics is needed.

6. PLANS

Development and verification of the 3DVAR/MM5 system for daily forecasts for the Los Angeles basin will continue in several ways.

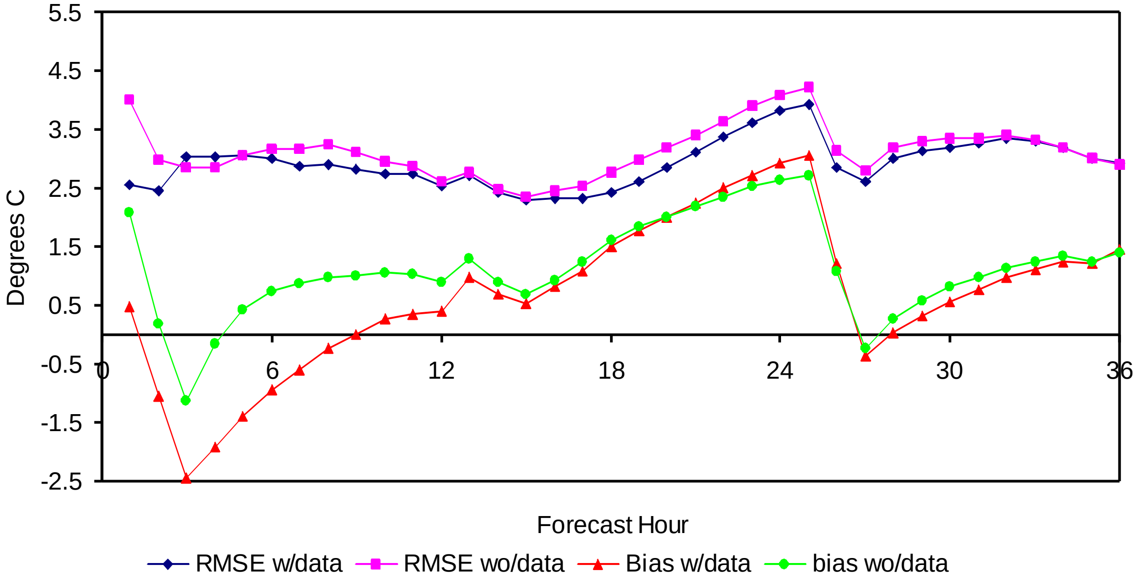
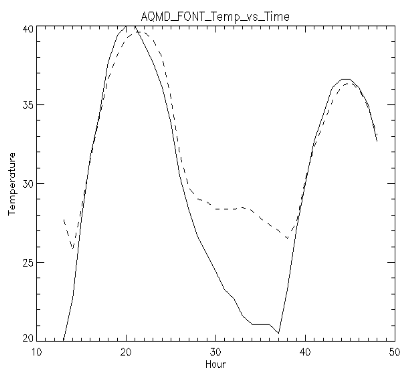
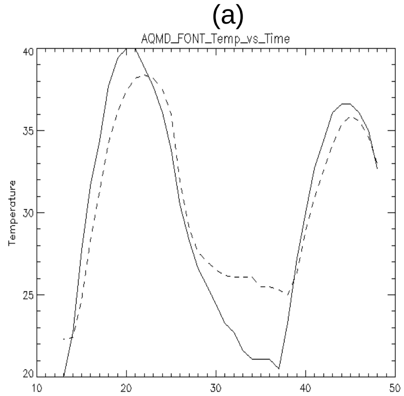


Figure 3. Hourly Root Mean Squared 2-meter temperature forecast error and bias using AQMD surface stations as truth data for the with (w/data) and without (wo/data) local data assimilation cases.



(a)



(b)

Figure 4. Time series of predicted (dashed line) and observed (solid line) at Fontana CA for the without (a) and with (b) local data assimilation cases

The first priority is to determine the cause of the high surface wind speed bias in the with data assimilation cases. Verification of both cases against non-surface observations is also needed to determine the complete impact of data assimilation on the quality of model forecasts. In terms of system improvements, we plan to implement a continual data assimilation cycle. Using this approach, one hopes to eliminate the loss of fine-scale flows that can occur when ETA analyses are used as a background for the domains. New data sources will also be assimilated such as Quikscat ocean surface winds and radar data. In addition, refined estimates of the background error fields will also be incorporated into the system.

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