The Impact of Nudging in the Meteorological Model for Retrospective Air Quality Simulations. Part I: Evaluation against National Observation Networks

TANYA L. OTTE

Atmospheric Sciences Modeling Division, NOAA/Air Resources Laboratory,* Research Triangle Park, North Carolina

ABSTRACT

It is common practice to use Newtonian relaxation, or nudging, throughout meteorological model simulations to create "dynamic analyses" that provide the characterization of the meteorological conditions for retrospective air quality model simulations. Given the impact that meteorological conditions have on air quality simulations, it has been assumed that the resultant air quality simulations would be more skillful by using dynamic analyses rather than meteorological forecasts to characterize the meteorological conditions, and that the statistical trends in the meteorological model fields are also reflected in the air quality model. This article, which is the first of two parts, demonstrates the impact of nudging in the meteorological model on retrospective air quality model simulations. Here, meteorological simulations are generated by the fifth-generation Pennsylvania State University–National Center for Atmospheric Research Mesoscale Model (MM5) using both the traditional dynamic analysis approach and using forecasts for a summertime period. The resultant fields are then used to characterize the meteorological conditions for emissions processing and air quality simulations using the Community Multiscale Air Quality (CMAQ) Modeling System. As expected, on average, the near-surface meteorological fields show a significant degradation over time in the forecasts (when nudging is not used), while the dynamic analyses maintain nearly constant statistical scores in time. The use of nudged MM5 fields in CMAQ generally results in better skill scores for daily maximum 1-h ozone mixing ratio simulations. On average, the skill of the daily maximum 1-h ozone simulation deteriorates significantly over time when nonnudged MM5 fields are used in CMAQ. The daily maximum 1-h ozone mixing ratio also degrades over time in the CMAQ simulation that uses MM5 dynamic analyses, although to a much lesser degree, despite no aggregate loss of skill over time in the dynamic analyses themselves. These results affirm the advantage of using nudging in MM5 to create the meteorological characterization for CMAQ for retrospective simulations, and it is shown that MM5-based dynamic analyses are robust at the surface throughout 5.5-day simulations.

1. Introduction

For two decades, limited-area Eulerian (or gridded) air quality models have been forced by meteorological fields that are generated by Eulerian meteorological models, in part, because meteorological observations and archived forecast fields do not exist at high enough temporal and spatial resolutions to capture atmospheric variables (e.g., mixing depth, column temperature, and wind profiles) that are important for regional-scale chemical transport modeling. Meteorological models such as the fifth-generation Pennsylvania State University–National Center for Atmospheric Research Mesoscale Model (MM5) and the Regional Atmospheric Modeling System (RAMS) have been able to bridge the gap by providing fields at the desired temporal and spatial resolutions. The accuracy of the modeled meteorological fields can be improved for retrospective simulations by creating "dynamic analyses" (Seaman et al. 1995) where Newtonian relaxation is applied throughout the simulation period. The dynamic analysis technique has also extended the run time over which modeled meteorological fields can be created and used without reinitializing to a period of several days or longer for air quality modeling applications.

Newtonian relaxation or "nudging" (Stauffer and

Corresponding author address: Tanya L. Otte, NOAA/Atmospheric Sciences Modeling Division, U.S. EPA Mail Drop E243-03, 109 T. W. Alexander Dr., Research Triangle Park, NC 27711. E-mail: tanya.otte@noaa.gov

Seaman 1990, 1994; Stauffer et al. 1991) is one method of four-dimensional data assimilation that is implemented in MM5, RAMS, and the Weather Research and Forecasting (WRF) Model. Nudging involves adding an artificial forcing term to the governing equations that reflects the difference between the best estimate of the observed state and the model state at a given location and time. The nudging term is weighted by a coefficient that is selected so that its reciprocal value represents the e-folding time (typically ~1 h for mass and momentum and ~1 day for moisture) over which the model error would be reduced in the absence of any other model forcing, and it is at least one order of magnitude smaller than the dominant terms in the equations. Nudging can be applied to horizontal wind components, temperature, and water vapor mixing ratio in any combination and with independent nudging coefficients. Nudging can be accomplished by using either gridded analyses of meteorological state variables where there is a "true" observed state at each model grid point (i.e., "analysis nudging") or by using high-frequency and/or high-density observations as they occur in space and time (i.e., "observation nudging").

It is well-known that using nudging in the meteorological model to create a dynamic analysis will lead to improved meteorological simulations (e.g., Stauffer et al. 1993; Seaman et al. 1995). It has been speculated that error accumulation in a regional-scale meteorological model in the absence of nudging can be so great after only 48 h that the resultant fields will have limited utility for air quality modeling applications because the simulated fields deviate significantly from the observations, so nudging should be particularly beneficial in dynamic analyses that are longer than 48 h (Seaman 2000). Dynamic analyses from sophisticated meteorological models (e.g., MM5) are typically used to generate multiday meteorological simulations that provide meteorological characterization for the Community Multiscale Air Quality (CMAQ) modeling system (Byun and Schere 2006) and other Eulerian air quality models for retrospective research and regulatory air quality modeling simulations.

Because the influence of the input meteorological fields on the air quality model simulation can be significant (e.g., Seaman 2000; Russell and Dennis 2000), one may expect that using improved meteorological fields from dynamic analyses in the chemistry–transport model (as opposed to using diagnostic or forecast meteorological fields) will lead to an improved air quality simulation. Barna and Lamb (2000) used observation nudging in MM5 and demonstrated that it improved ozone predictions in the complex terrain of the Pacific Northwest with the "CALGRID" model over a 4-day

period. Tanrikulu et al. (2000) showed that nudged meteorological fields improved ozone predictions by a regional air quality model during a 4-day ozone episode in the San Joaquin Valley of California. Umeda and Martien (2002) used nudging in RAMS and performed tracer simulations using a Lagrangian particle model (LPM) and ozone simulations using the Urban Airshed Model (UAM-V) in the episode simulated by Tanrikulu et al. (2000). Umeda and Martien (2002) found that nudged meteorological fields improved the LPM simulations of tracer concentrations, but nudged (rather than forecast) meteorological fields did not improve UAM-V ozone predictions. Umeda and Martien (2002) concluded that the uncertainty in other inputs to the air quality modeling system (e.g., emissions inputs and chemical boundary conditions) may minimize the influence of the nudging on the UAM-V simulation. In addition, both Barna and Lamb (2000) and Umeda and Martien (2002) concede that their results only represent a brief modeling period, and so those results (which are contradictory) may not be general. In an effort to more conclusively establish the impact of nudging in the meteorological model on air quality simulations, longer-term air quality simulations (i.e., more than one-week duration) with state-of-the-science meteorological and air quality models are evaluated in this study. Understanding and establishing the value of nudging in the meteorological model for the air quality simulation can be important to identify sensitivities and to define how errors in meteorological fields impact simulated pollutant transport and fate. In addition, there could be implications for defining the optimal continuous simulation length for the meteorological model as well as optimal air quality forecast periods. Furthermore, this research can improve the methodology used to create dynamic analyses, and it can help to focus areas of improvement in meteorological modeling to support air quality applications.

This paper is the first of two parts that quantify the impact of nudging in the meteorological model on the air quality simulation. Here the focus is on broad evaluation against independent meteorological and air quality observation networks that have dense national coverage by comparing simulations for a 35-day summer period; using the same simulations, Otte (2008, hereinafter Part II) focuses on evaluation against collocated meteorological and air quality measurements to gain insight into behavior of meteorological and photochemical fields at individual observation sites. Section 2 describes the meteorological, emissions, and air quality model configurations. Section 3 includes analysis of the MM5 and CMAQ simulations showing the impact with

and without nudging in MM5. The final section provides a discussion of the conclusions.

2. Model configuration

The meteorological, emissions, and air quality modeling suite is run for two configurations of input meteorological conditions: one that uses analysis nudging throughout the simulation (i.e., a dynamic analysis for retrospective air quality modeling), and one that does not (i.e., effectively using forecast fields for air quality modeling). The simulations are performed on a domain with 36-km horizontal grid spacing that includes the continental United States and parts of Canada and Mexico. Thirty-four terrain-following layers are used for both the meteorological and air quality simulations; there is no "collapsing of layers" or reduction of vertical resolution in the air quality model, as is commonly done (e.g., Eder and Yu 2006; Hogrefe et al. 2006). There are 18 layers in the lowest 2 km of the atmosphere for the meteorological and air quality simulations.

MM5 (Grell et al. 1994), version 3.6, is used for the meteorological simulations. The background fields and lateral boundary conditions for MM5 originate from the National Centers for Environmental Prediction (NCEP) North American Mesoscale (NAM) Model (i.e., for this period, the Eta Model; Black 1994) 3-h analyses. The physics options used in MM5 in this study include the Rapid Radiative Transfer Model (RRTM; Mlawer et al. 1997) for longwave radiation, the Dudhia shortwave radiation scheme (Grell et al. 1994), the Kain–Fritsch 2 convective model (Kain 2004), the Reisner 2 microphysics parameterization (Reisner et al. 1998), the Asymmetric Convective Model (ACM) for the planetary boundary layer (PBL; Pleim and Chang 1992), and the Pleim–Xiu land surface model (LSM; Xiu and Pleim 2001). In the MM5 simulation that includes nudging, 3-h 3D analyses of temperature, water vapor mixing ratio, and horizontal wind components influence the simulation with nudging coefficients of 3.0×10^{-4}, 1.0×10^{-5}, and 3.0×10^{-4} s^{-1}, respectively. Three-hourly surface analyses of horizontal wind components are also used with a nudging coefficient of 3.0×10^{-4} s^{-1}. There is no nudging of mass fields at the surface or within the PBL (e.g., Stauffer et al. 1991).

The MM5 simulation that does not include nudging cannot be considered a true forecast; rather it is a pseudoforecast for purposes of this research. That MM5 simulation contains two primary advantages over traditional forecasts. First, the lateral boundary conditions originate from NAM Model analyses, which are assumed to be superior to the NAM Model forecasts

that likely would be used if MM5 were run strictly as a forecast. Using analyses rather than forecasts to force the lateral boundaries in MM5 should serve to improve the meteorological fields, particularly as the simulation run time increases. Second, the Pleim–Xiu LSM is run using the soil moisture nudging option (Pleim and Xiu 2003), which can mitigate the effects on soil moisture (and, hence, surface sensible and latent heat fluxes) of poorly forecasted precipitation. Although the soil moisture nudging uses near-surface meteorological analyses to indirectly adjust the surface fluxes in the LSM, it is not part of the direct forcing in the dynamic analysis procedure. The soil moisture nudging is an integral part of the Pleim–Xiu LSM for retrospective air quality modeling, and the option is employed in the nonnudged MM5 simulation so that it does not have a secondary disadvantage as compared with the dynamic analyses. Furthermore, in the absence of a sophisticated soil moisture initialization scheme, using the Pleim–Xiu LSM without soil moisture nudging is likely to adversely impact the skill of the mesoscale model, particularly for near-surface temperature (Pleim and Xiu 2003), which is important for emissions and deposition processes that directly affect air quality predictions. The purpose of this research is strictly to evaluate the impact of using dynamic analyses on the resulting air quality simulation, so the lateral boundary conditions and the LSM are configured to be the same in both MM5 simulations. Using a typical retrospective modeling configuration (except for analysis nudging) for the nonnudging MM5 simulation will improve its skill over a true forecast.

The emissions are based on the U.S. Environmental Protection Agency (EPA) 2001 National Emission Inventory. The emissions are processed using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Houyoux et al. 2000), version 2.2. Mobile source emissions are processed with the "MOBILE6" (Environmental Protection Agency 2003) model within SMOKE using climatological temperatures. The biogenic emissions are processed using the Biogenic Emissions Inventory System, version 3 (BEIS3; Pierce et al. 1998). For this work, the biogenic and point-source emissions sectors are reprocessed for each MM5 simulation to capture the effects of the hourly meteorological fields on the emissions. All other emissions sectors are independent of the MM5 simulations.

Air quality is modeled using CMAQ (Byun and Schere 2006), version 4.6. The 2005 update to the Carbon Bond chemical mechanism (CB05; Yarwood et al. 2005; Sarwar et al. 2008) is used. The PBL is modeled using the ACM, version 2 (ACM2; Pleim 2007). The fourth version of the Modal Aerosol Model (AERO4;

TABLE 1. Dates in 2001 used for analysis as given by time elapsed within each MM5 run segment. MM5 segments 1 and 2 are part of the CMAQ spinup period, and they are not included in the analysis.

MM5 segment	Day 1	Day 2	Day 3	Day 4	Day 5
3	30 Jun	1 Jul	2 Jul	3 Jul	4 Jul
4	5 Jul	6 Jul	7 Jul	8 Jul	9 Jul
5	10 Jul	11 Jul	12 Jul	13 Jul	14 Jul
6	15 Jul	16 Jul	17 Jul	18 Jul	19 Jul
7	20 Jul	21 Jul	22 Jul	23 Jul	24 Jul
8	25 Jul	26 Jul	27 Jul	28 Jul	29 Jul
9	30 Jul	31 Jul	1 Aug	2 Aug	3 Aug

Binkowski and Roselle 2003) is used for aerosol dynamics. Chemical dry deposition velocities are computed using an electrical analog resistance model (M3DRY; Pleim et al. 2001). The chemistry lateral boundary conditions are prepared from a global simulation using the "GEOS-CHEM" model (Bey et al. 2001).

The MM5 simulations are run for the period 1200 UTC 19 June–0000 UTC 4 August 2001. The period is broken into nine overlapping 5.5-day run segments. The first 12 h of each MM5 segment are a "spinup" period for cloud processes, and they are not used for emissions or chemistry processing; the remaining 5 days are input for the air quality model. All fields except soil moisture are reinitialized in each MM5 segment, as is typically done for retrospective modeling applications of CMAQ. The CMAQ simulations cover the period 0000 UTC 20 June–0000 UTC 4 August 2001, but the first 10 days are considered spinup to allow the chemistry to come into equilibrium, and they are not included in the analysis.

3. Analysis

Two sets of MM5 and CMAQ simulations for the 35-day period 30 June–3 August 2001 are analyzed to assess the impact of using nudging in MM5 on the CMAQ simulation. This time period is selected because it is in the middle of the ozone season, which is typically May–September in most areas of the United States, when high levels of pollutants are typically observed. The first set of simulations (NONUDGE) is composed of overlapping 5.5-day "forecasts" that do not include analysis nudging in MM5. The second set of simulations (NUDGE) includes overlapping 5.5-day dynamic analyses that are prepared in the traditional manner as input to CMAQ for retrospective air quality modeling studies. The 35-day period includes seven MM5 run segments (see Table 1). Because the skill of the meteo-

rological models degrades over time, particularly in the absence of nudging, the model performance (MM5 and CMAQ) is aggregated over time slices within each 5.5-day MM5 run segment (Table 1). Because the first 12 h of each MM5 run segment is not used, "day 1" refers to hours 13–36 of the MM5 run segment, "day 2" refers to hours 37–60, and so on. The CMAQ performance is binned in time, as well, to determine the impact on the chemistry–transport model as it corresponds to increased simulation run time in MM5. Statistics are computed for near-surface meteorological fields and near-surface daily maximum 1-h ozone using metrics defined by Willmott (1982) and as applied in Otte et al. (2004).

a. Meteorological fields

The MM5 performance is assessed for the two simulations using a standard suite of statistical measures by comparing with near-surface meteorological observations collected by the National Weather Service (NWS). This analysis is performed to gauge the relative improvement in the surface meteorological fields, which greatly impact near-surface air quality modeling, when nudging is used in MM5. No upper-air meteorological evaluation is performed in this study because there is no analogous comparison with upper-air air quality observations, and it is well known that a dynamic analysis with MM5 is generally statistically superior to a forecast (e.g., Stauffer et al. 1993; Seaman et al. 1995). It should be noted that the near-surface wind analyses are used in NUDGE, and many of the NWS observations that are part of the evaluation below are incorporated into the NAM Model analyses toward which MM5 is forced in NUDGE. Those NAM Model analyses, however, have been interpolated twice (via NCEP postprocessing to the distributed domain and via MM5 preprocessing to the horizontal domain used here) before being ingested for nudging, so the influence of the individual observations in their MM5 grid cells is diminished. The analyses of near-surface temperature and near-surface moisture are not used in the dynamic analysis process in NUDGE (see Stauffer et al. 1991), so those data can be considered independent for evaluation. However, near-surface temperature and moisture analyses are used in both NUDGE and NONUDGE to indirectly force the soil moisture as part of the Pleim–Xiu LSM in MM5 (Pleim and Xiu 2003).

Figure 1 shows the mean absolute error (MAE), index of agreement (IA), and mean bias error (MBE) for 2-m temperature and 10-m wind speed calculated against all NWS surface stations in the MM5 domain and binned by day within each MM5 run segment (see Table 1). Figure 1 indicates that the MAE, IA, and MBE statistics for 2-m temperature and 10-m wind
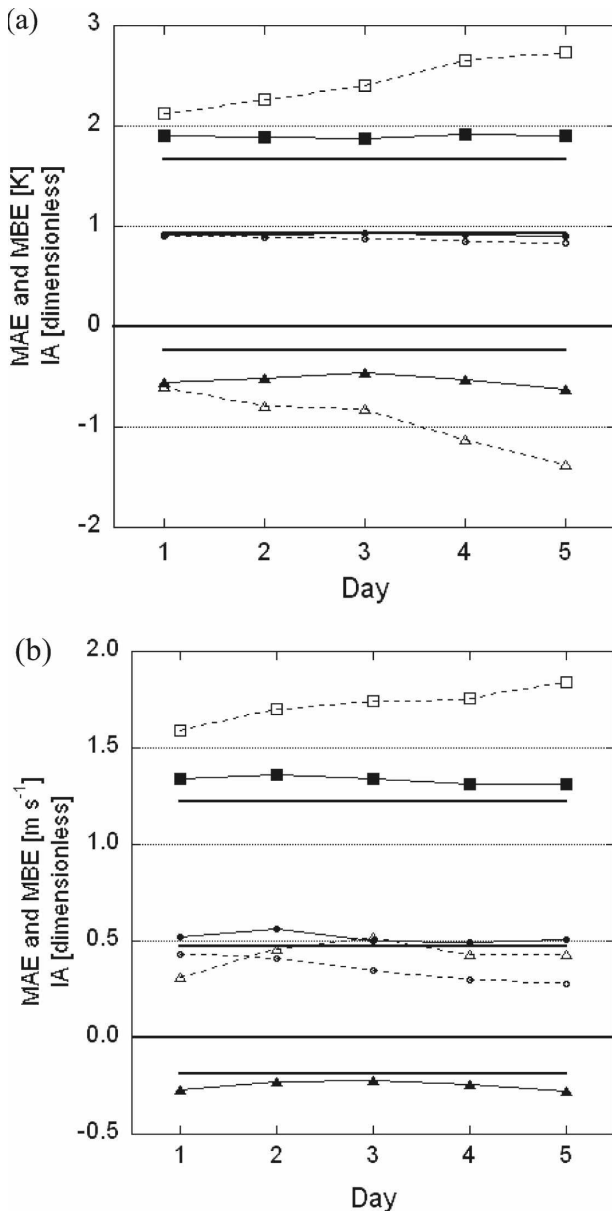
FIG. 1. Statistics "by day" within the MM5 simulation for the period 30 Jun–3 Aug 2001 computed at NWS sites. Solid lines with closed symbols represent NUDGE. Dashed lines with open symbols represent NONUDGE. Thick solid lines are statistics for a 3-month summer period (June, July, and August 2001) in a similar MM5 simulation as reported in Gilliam et al. (2006). Squares represent MAE (SI units), circles represent IA (dimensionless), and triangles represent MBE (SI units); (a) 2-m temperature in K and (b) 10-m wind speed (m s⁻¹).

speed in the NUDGE simulation over the 35-day period are comparable to those computed for dynamic analyses for the full summer (June, July, and August) over the same domain and year and using a similar MM5 configuration (Gilliam et al. 2006), so it can be

concluded that the seven MM5 run segments used here are representative of the same summer period. The MM5 simulation, NUDGE, performs with reasonable consistency through the MM5 segment (i.e., little change in statistical skill with increased simulation time), as seen in the MAE, IA, and MBE in Fig. 1. However, the MM5 simulation without the nudging, NONUDGE, shows a marked decrease in skill with increased run time, as expected. Figure 1a shows that the MAE for 2-m temperature in NUDGE is, on average, maintained at ~1.9 K for each day within the MM5 run segment, but MAE increases steadily from 2.1 to 2.7 K in NONUDGE. This results in an average improvement of 0.23 K in day 1 that increases to 0.84 K across the simulation domain by day 5. Similarly MBE for 2-m temperature fluctuates mildly between −0.46 and −0.62 K in NUDGE, while the cold bias grows from −0.60 on day 1 to −1.37 by day 5 in NONUDGE. The IA (which is bounded between 0 and 1, where IA = 1 is a perfect model) for 2-m temperature in NUDGE ranges from 0.91 to 0.93 when aggregated by day over the 35-day period, while it gradually decreases from 0.90 to 0.83 in NONUDGE as the MM5 simulation run time increases.

The statistical trends for 10-m wind speed (Fig. 1b) are similar to those shown for 2-m temperature. The MAE for 10-m wind speed gently oscillates from 1.31 to 1.36 m s⁻¹ for days 1–5 in NUDGE, while MAE steadily increases from 1.59 to 1.84 m s⁻¹ in NONUDGE. This suggests that, on average, using nudging in MM5 for this summer period results in an improvement in MAE for 10-m wind speed of 0.25 m s⁻¹ in day 1 that increases to 0.53 m s⁻¹ by day 5, relative to MM5 forecasts for the same time period. Likewise, the MBE for 10-m wind speed is fairly constant (from −0.23 to −0.27 m s⁻¹) as the simulation run time increases in NUDGE, whereas it is larger and more variable (0.31–0.52 m s⁻¹) in NONUDGE. The IA for 10-m wind speed also remains somewhat constant in NUDGE (0.50–0.56), while it steadily decreases from 0.43 to 0.28 in NONUDGE.

Figure 2 shows the diurnal variation of MAE across the full simulation domain by day within the MM5 run segment (Table 1) for four near-surface variables. For 2-m temperature (Fig. 2a), 2-m water vapor mixing ratio (Fig. 2b), 10-m wind speed (Fig. 2c), and 10-m wind direction (Fig. 2d), a similar diurnal pattern of MAE is observed for each of the five days (similar range of values and amplitude through the diurnal cycle), and there is no discernable change in skill from day 1 to day 5 (consistent with Fig. 1). However, in NONUDGE, there is a general increase in MAE (i.e., decline in skill) from day 1 to day 5 for each of the four near-surface
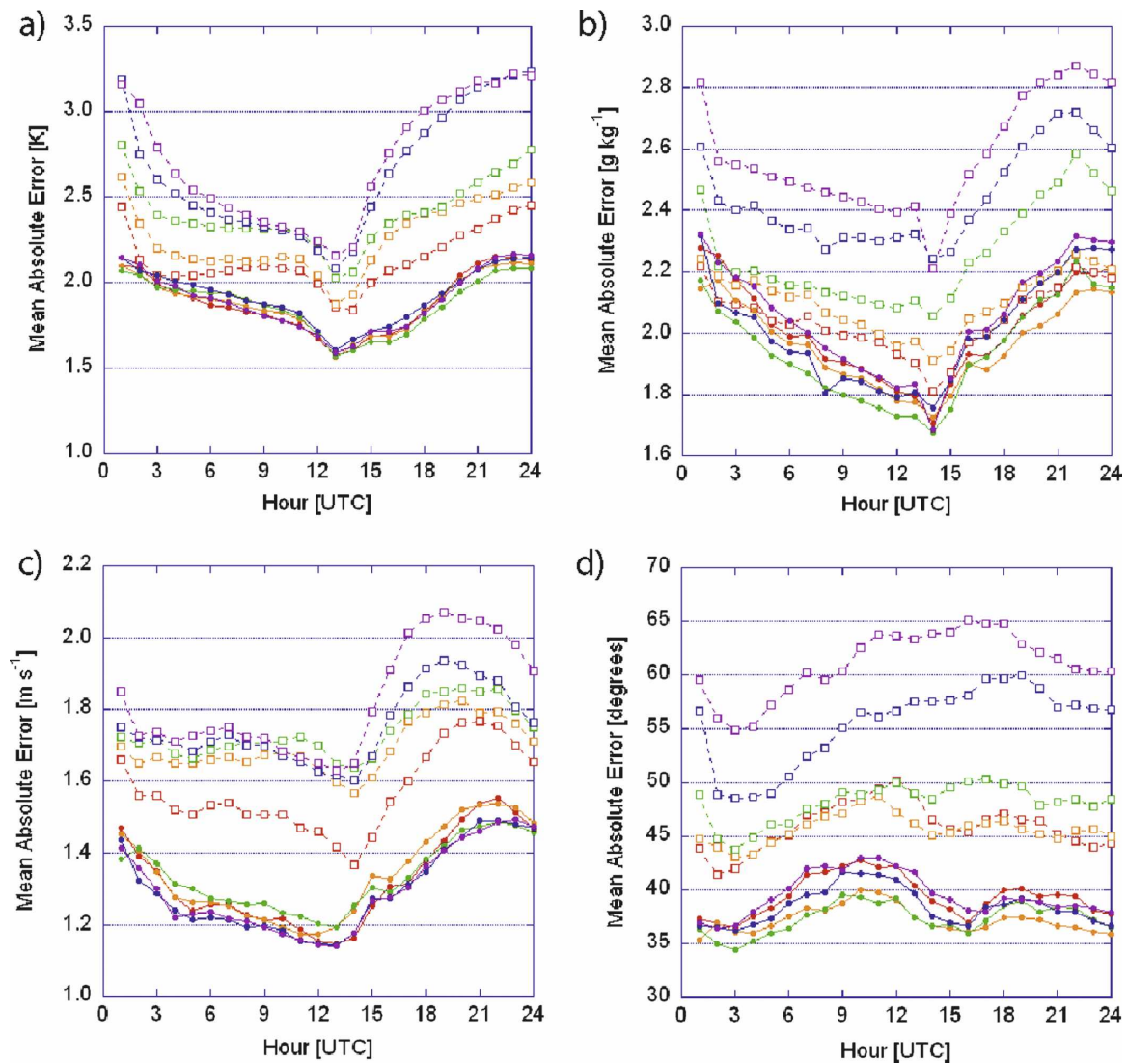
FIG. 2. Diurnal variation of MAE for near-surface meteorological variables at NWS observation sites throughout the 36-km domain, plotted "by day" within the meteorological simulation for the period 30 Jun–3 Aug 2001. Statistics from NUDGE are shown as filled circles connected by solid lines, and NONUDGE are open squares connected by dashed lines. Color coding represents days within MM5 simulation: day 1 is red, day 2 is orange, day 3 is green, day 4 is blue, and day 5 is purple; (a) 2-m temperature, (b) 2-m water vapor mixing ratio, (c) 10-m wind speed, and (d) 10-m wind direction.

meteorological fields. On average, the MAE is almost always higher (i.e., showing lower skill) at all hours of the day in NONUDGE than in NUDGE for the four near-surface variables shown in Fig. 2. The range and amplitude (i.e., the difference between maximum and minimum hourly values in the diurnal cycle depicted in Fig. 2) of MAE over the hours of the day both tend to increase with increased simulation run time in NONUDGE for all four near-surface variables. For example, Fig. 2a shows that day 1 MAE for 2-m temperature in NONUDGE ranges from 1.84 to 2.45 K (which leads to an amplitude of 0.61 K), but by day 5, MAE

ranges from 2.16 to 3.23 K (amplitude of 1.07 K). The same relative comparison is also true for 2-m water vapor mixing ratio (Fig. 2b), 10-m wind speed (Fig. 2c), and 10-m wind direction (Fig. 2d), but with smaller relative increases in amplitude. In general, the largest MAE for 2-m temperature, 2-m water vapor mixing ratio, and 10-m wind speed in both NUDGE and NONUDGE occur in the afternoon (i.e., approximately 1800–0000 UTC, depending on location within the United States) when the PBL is deepest. In NONUDGE, the MAE during the PBL growth period grows at a greater rate than during other parts of the day. Therefore, the errors
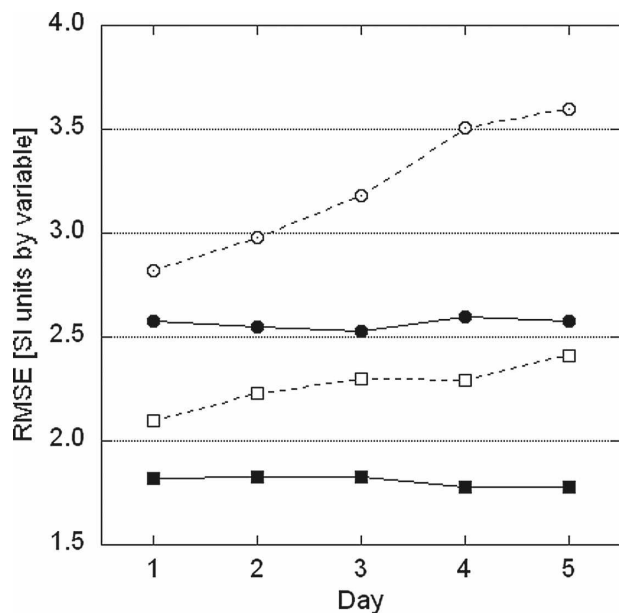
FIG. 3. Comparison of rmse for MM5 simulations at NWS sites by day within the MM5 simulation for the period 30 Jun–3 Aug 2001. Solid lines with closed symbols represent NUDGE. Dashed lines with open symbols represent NONUDGE. Circles represent 2-m temperature, and squares represent 10-m wind speed.

in CMAQ-simulated ozone, which typically reaches its peak mixing ratio in late afternoon (e.g., Otte et al. 2005), in NONUDGE may be accentuated by the decline in meteorological modeling skill during the PBL growth period.

Figure 3 shows the root-mean-square error (rmse) for 2-m temperature and 10-m wind speed calculated against all NWS surface stations in the MM5 domain and binned by day (following Table 1) for NONUDGE and NUDGE. As with the statistical measures presented in Fig. 1, on average, the rmse for NUDGE remains fairly constant throughout the MM5 simulation period, while the rmse tends to increase with increased simulation run time in NONUDGE. The 2-m temperature rmse in NUDGE ranges from 2.55 to 2.60 K for each of the 5 days, while it rises from 2.82 to 3.60 K over the same time period in NONUDGE. On average, the rmse for 10-m wind speed is ~1.8 m s^{-1} on each of the 5 days in NUDGE, but it grows from 2.1 to 2.4 m s^{-1} in NONUDGE. The steeper growth of the rmse for 2-m temperature and 10-m wind speed over time (comparing day 1 to day 5) in NONUDGE compared with MAE (Fig. 1) suggests that there may be more variability (i.e., outliers) as the MM5 simulation run time increases.

The statistics shown in Figs. 1, 2, and 3 confirm that using analysis nudging in MM5 to create dynamic analyses generates more accurate meteorological fields

than forecasts. On average, there is little change in statistical skill over the 5.5-day period in MM5 when nudging is used to generate dynamic analyses (i.e., in NUDGE), whereas there is a considerable decrease in skill with increased simulation run time in the absence of forcing toward analyses (i.e., in NONUDGE). On average, there is no discernable loss of skill within the diurnal cycle for the 5.5-day MM5 dynamic analyses. Therefore, MM5 dynamic analyses that are generated with the options used herein are robust near the surface for at a least 5.5-day simulation at 36-km horizontal grid spacing.

b. Air quality

Because of the temporal binning used in this analysis, it is necessary to compare with air quality observations that are available with a high temporal frequency (i.e., no coarser than daily) and a high spatial coverage. There are only a few air quality observation networks available in the United States (e.g., Eder and Yu 2006), but only one network meets the requirements for the initial comparison. Therefore, the CMAQ simulations are compared with surface hourly ozone and daily maximum 1-h ozone observations from the U.S. EPA's Air Quality System (AQS) database. More than 1000 ozone monitors are part of the AQS database, and the highest observation densities are in the eastern United States (east of the Mississippi River) and California (refer to Fig. 5). The AQS monitors are typically located in and around urban centers where ozone historically has been observed at high levels that exceed the National Ambient Air Quality Standards (NAAQS).

Ozone is selected for evaluation in this study because it is one of the pollutants for which the EPA has established the NAAQS, and ozone is currently the only pollutant for which widespread hourly and daily measurements exist. From 1978 to 1997, the EPA maintained a standard for ozone that the fourth-highest daily maximum 1-h ozone mixing ratio over a 3-year period shall not exceed the NAAQS level of 0.12 ppm. The NAAQS for ozone was updated in 1997 to use a daily maximum 8-h average of 0.08 ppm rather than the maximum 1-h mixing ratio standard. Hogrefe et al. (2001) note that the intraday fluctuations in daily maximum ozone prediction increase the inherent uncertainty due to the model's inability to adequately characterize subgrid processes. However, the maximum 1-h standard provides a reasonable benchmark for model performance (e.g., Biswas and Rao 2001; Sistla et al. 2001; Eder and Yu 2006), albeit perhaps a more challenging field than the maximum 8-h average. Biswas and Rao (2001) received comparable model per-

formance when evaluating two modeling systems with both the 1- and 8-h standards.

The air quality module of the Atmospheric Model Evaluation Tool (AMET; Gilliam et al. 2005; K. W. Appel 2006, personal communication) is used for computing model–observation matching statistics. It is acknowledged that this comparison is not exact because the observations reflect point measurements while the CMAQ-based simulations are volume-average ozone mixing ratios, but this technique is commonly employed for air quality model evaluation (e.g., Sistla et al. 2001; Eder and Yu 2006). It should be noted that the AQS observations are recorded from midnight to midnight, local standard time (LST), and the MM5 and CMAQ simulation days are defined for this study using coordinated universal time. The air quality module of AMET stores the model–observation pairs in terms of LST (which is the standard time convention for air quality observations), so all model–observation pairings are made for "days" in LST. Therefore, in the analysis of the CMAQ simulations shown below, the day bins cannot be exactly compared with the data shown for MM5. This issue can be important for AQS sites in California, where MM5–CMAQ days are 1600 to 1600 LST on the following day, which may not include the daily maximum 1-h surface ozone that corresponds to the calendar day. In the eastern United States, the daily maximum 1-h surface ozone is often within the same day using either UTC or LST, so it is less of an issue there. Further inspection of the data is required to determine the impact of this time-matching idiosyncrasy on the interpretation of the results. To minimize the effect of the time-matching issue as well as the reduced representativeness of 36-km modeled output at point measurements in the complex terrain of the western United States, comparisons between CMAQ simulations and AQS sites are restricted to sites east of 100°W longitude in this paper. However, the statistical trends for daily maximum 1-h ozone shown "by day" within the MM5 simulation are similar when computed for all AQS sites throughout the United States (see Fig. 5).

Figure 4a shows the rmse for the surface daily maximum 1-h ozone and its systematic (rmses) and unsystematic (rmseu) vector components (Willmott 1982) for AQS sites east of 100°W longitude. The rmses accounts for processes that the model does not simulate well and can be improved, whereas the rmseu can be attributed to subgrid-scale processes that are not adequately characterized by the modeling system, measurement error, or random error. The CMAQ simulation that uses input meteorological fields from NUDGE tends to be a better overall simulation for maximum 1-h ozone than the simulation that uses meteorological fields from
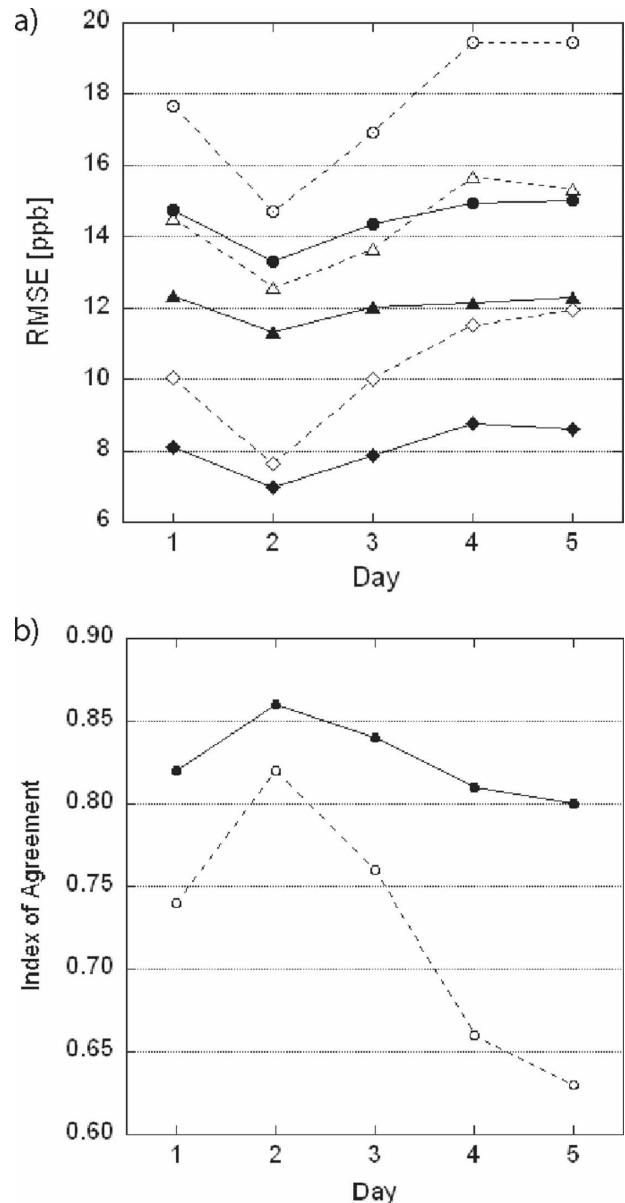

FIG. 4. Statistics by day within the MM5 simulation for the period 30 Jun–3 Aug 2001. Solid lines with closed symbols represent NUDGE. Dashed lines with open symbols represent NONUDGE. (a) Comparison of rmse for CMAQ simulations at AQS sites east of 100°W. Circles represent total rmse for daily maximum 1-h ozone, diamonds represent rmses for daily maximum 1-h ozone, and triangles represent rmseu for daily maximum 1-h ozone. (b) Comparison of IA for CMAQ simulations at AQS sites east of 100°W.

NONUDGE, as reflected in the total rmse and in both the rmses and the rmseu, which are all lower on average by day for NUDGE relative to NONUDGE. The rmseu does not exhibit a substantial change through the MM5 run segment for NUDGE (varies by ~1 ppb over the 5-day bins), but it varies by more than 3 ppb in
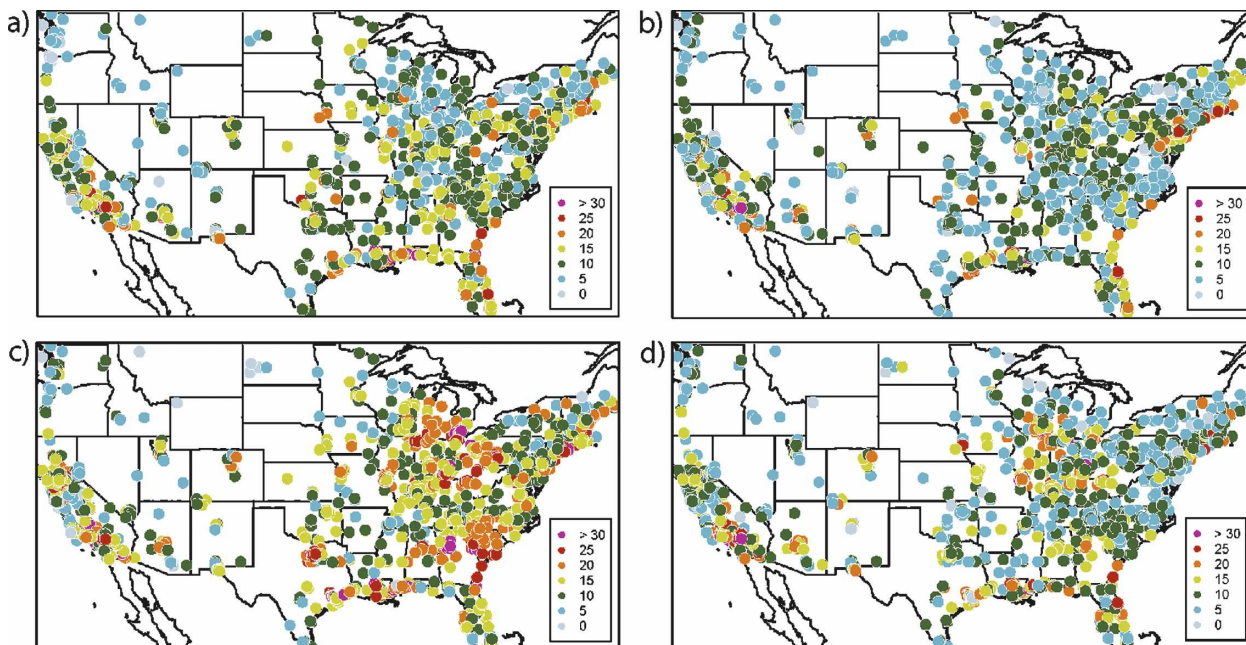
FIG. 5. Rmse for maximum 1-h ozone in ppb at AQS sites for (a) day 2 NONUDGE, (b) day 2 NUDGE, (c) day 5 NONUDGE, and (d) day 5 NUDGE.

NONUDGE. The rmses shows a steeper rate of change in NONUDGE than in NUDGE, particularly between days 2 and 5. The rmse suggests a marked decrease in skill and increases by 4.7 ppb between days 2 and 5 for NONUDGE. Somewhat surprisingly, there is also a gradual increase in rmse by 1.7 ppb for daily maximum 1-h ozone from day 2 to day 5 in NUDGE, which suggests a gradual decrease in skill concurrent with increased MM5 simulation run time. A similar trend for NUDGE is seen in both rmses and rmseu.

Figure 4b shows the IA for the surface daily maximum 1-h ozone in comparison with AQS sites east of 100°W longitude. When aggregated by day within the MM5 run segment, the IA varies slightly between 0.80 and 0.86 for NUDGE, while it has a much larger range (0.63–0.82) for NONUDGE. The IA follows a similar trend from day 1 to day 5 for NUDGE and NONUDGE, where the peak performance for daily maximum 1-h ozone occurs on day 2 within the MM5 run segment, followed by a steady decline in skill from day 2 to day 5. The behavior of the IA for NUDGE and NONUDGE is similar to the behavior of rmse (Fig. 4a). Like the rmse (Fig. 4a), the IA also shows a more rapid degradation of skill over time within the MM5 simulation in NONUDGE as compared with NUDGE. Also, like rmse, the IA shows a decline in skill with time in NUDGE that is not reflected in the near-surface meteorological variables (Figs. 1, 2, and 3).

Figure 5 shows spatial comparisons of rmse for daily maximum 1-h ozone for days 2 and 5 for the CMAQ simulations that used MM5 fields generated by NONUDGE and NUDGE. Figure 5a shows that the day 2 CMAQ simulations with meteorological input from NONUDGE typically have widespread rmse of 5–20 ppb. The day 2 CMAQ simulations with meteorological input from NUDGE (Fig. 5b) indicate slightly smaller rmse, often 5–15 ppb. Figures 5a and 5b illustrate a fairly consistent spatial improvement in CMAQ ozone predictions by using nudging in MM5, as early as day 2. By day 5, the CMAQ simulation that used meteorological input from NONUDGE (Fig. 5c) experiences a widespread decrease in statistical skill relative to both the day 5 NUDGE (Fig. 5d) and to the day 2 NONUDGE. The rmse in day 5 NONUDGE are generally 10–30 ppb, as compared with rmse of 5–20 ppb in day 5 NUDGE. Figures 5b and 5d show that the gradual decrease in statistical skill over time for daily maximum 1-h ozone with NUDGE (which is also seen in Fig. 4) is observed throughout the simulation domain.

The results in Figs. 4 and 5 suggest that using MM5 dynamic analyses (e.g., NUDGE) to characterize the meteorological fields for emissions processing and CMAQ model simulations is advantageous over pseudoforecasts (e.g., NONUDGE), as assessed by skill scores for daily maximum 1-h ozone. Interestingly, the trends for rmse (Fig. 4a) and IA (Fig. 4b) for daily maximum 1-h ozone do not parallel the trends for the

near-surface meteorological variables (Figs. 1, 2, and 3) in either NUDGE or NONUDGE. In both NUDGE and NONUDGE, the day 2 daily maximum 1-h ozone simulation clearly has better statistical skill scores than day 1 (Fig. 4), which are not observed for the near-surface meteorological variables. In fact, a subtle decline in statistical skill for daily maximum 1-h ozone can be seen in NUDGE as the meteorological simulation run time increases, where the statistical scores for the near-surface meteorological variables are fairly constant in time through the 5.5-day MM5 dynamic analyses.

Figure 6 shows the daily rmse and IA for daily maximum 1-h ozone at AQS sites east of 100°W longitude simulated by CMAQ for NUDGE and NONUDGE. The daily eastern domainwide rmse (Fig. 6a) within each of the seven MM5 run segments does not reveal the same aggregate trend in the statistics that is shown "by day" (Fig. 4a). This is not surprising because Hogrefe et al. (2006) note that one-way coupled Eulerian meteorological–photochemical modeling systems (e.g., MM5–CMAQ) have more difficulty capturing high-frequency intraday and diurnal variability than synoptic and seasonal fluctuations in temperature, wind speed, and ozone. However, it is interesting that the rmse decreases between day 1 and day 2, which suggests higher skill on day 2 than day 1, in six of the seven run segments in NONUDGE and by more than 1 ppb in five of those six run segments to as much as 8.3 ppb. The rmse is lower between day 1 and day 2 in four of the seven run segments in NUDGE by as much as 3.5 ppb, and the rmse increases by less than 0.5 ppb between day 1 and day 2 in two of the remaining three run segments in NUDGE. The daily IA for maximum 1-h ozone (Fig. 6b) follows a similar pattern to rmse, as it increases from day 1 to day 2 (indicating greater skill in day 2 than day 1) for four of the seven run segments in NUDGE and five of the seven run segments in NONUDGE.

At this time, only speculative explanation can be offered for the poorer skill for daily maximum 1-h ozone simulated by CMAQ on day 1 when compared with day 2 in most MM5 run segments for both NONUDGE and NUDGE. One possible cause for the gain in skill in day 2 in CMAQ is related to the ozone time scale. Rao et al. (1997) report that the time scale for ozone in the United States is on the order of 1–2.5 days, depending on the monitoring location; thus, it is unlikely that the statistical change between days 1 and 2 is related to a coincidental alignment of synoptic patterns, which are typically on a 5-day cycle, during the analysis period. Because both NUDGE and NONUDGE show a decline in skill in ozone predictions in CMAQ as the MM5 run time increases, there is an accumulation of error in
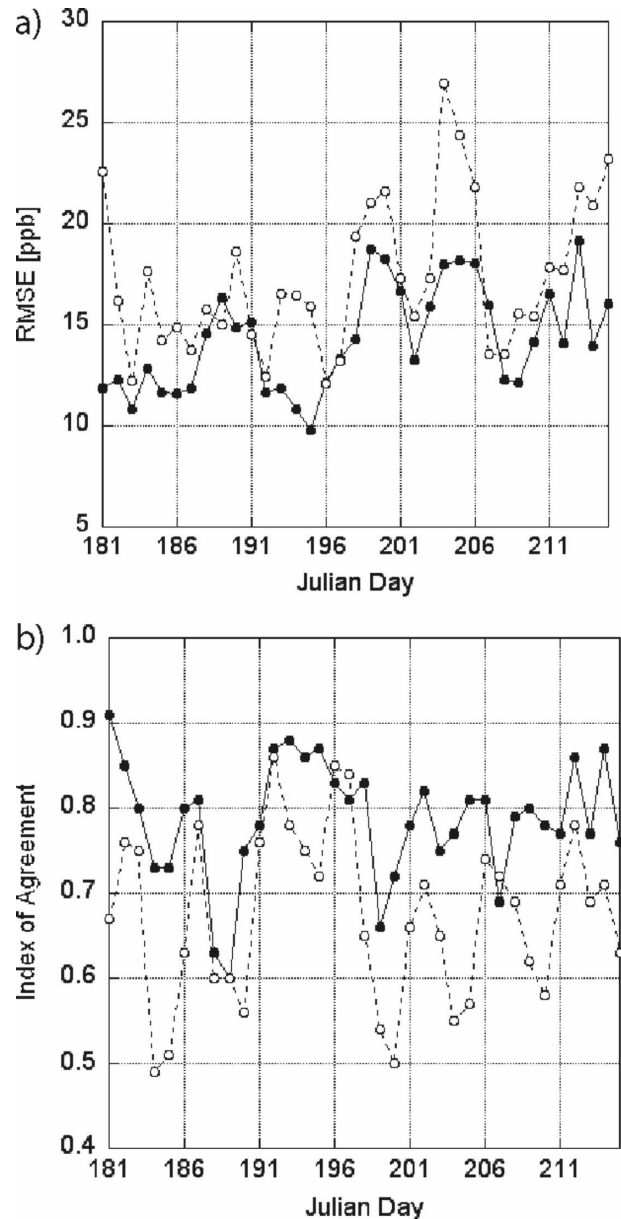

FIG. 6. Daily statistics for maximum 1-h ozone at AQS sites east of 100°W for the period 30 Jun (Julian day 181)–3 Aug (yearday 215) 2001. Day 1 within the MM5 run segment is indicated by a vertical line through the data points. Solid lines with closed symbols represent NUDGE. Dashed lines with open symbols represent NONUDGE; (a) rmse and (b) IA.

CMAQ over time. There is a physical discontinuity in the meteorological fields at the beginning of day 1 that is not replicated in the CMAQ chemical fields. (Recall that the CMAQ chemistry and lateral boundary conditions are continuous in time so no additional spinup of chemical processes takes place with a change of MM5 run segment.) It is also possible that the chemistry is no longer in balance at the beginning of day 1, perhaps
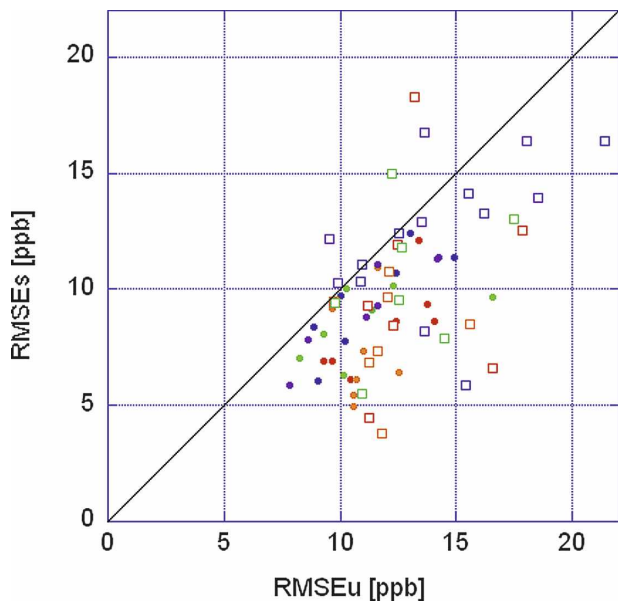
FIG. 7. Rmse and its systematic and unsystematic vector components for maximum 1-h ozone at AQS sites east of 100°W, plotted both daily and by day within the meteorological simulation for the period 30 Jun–3 Aug 2001. Rmse is represented by the length of the line from the origin to the symbol. Statistics from NUDGE are shown as filled circles, and NONUDGE are open squares. Color coding represents days within MM5 simulation: day 1 is red, day 2 is orange, day 3 is green, day 4 is blue, and day 5 is purple.

TABLE 2. Divisions (%) of systematic and unsystematic error by day within MM5 simulation for daily maximum 1-h ozone simulated by CMAQ in NONUDGE and NUDGE. SYS and UNSYS are adapted from Willmott (1982) and are defined as used here in Otte et al. (2004).

	NONUDGE		NUDGE	
	SYS	UNSYS	SYS	UNSYS
Day 1	32.5	67.5	30.2	69.8
Day 2	27.0	73.0	27.6	72.4
Day 3	34.9	65.1	29.9	70.1
Day 4	35.0	65.0	34.2	65.8
Day 5	37.7	62.3	33.0	67.0

because of instantaneous changes in clouds, precipitation, and meteorological state variables that result from stringing together reinitialized, overlapping MM5 run segments (e.g., at 0000 UTC 5 July, 0000 UTC 10 July, etc., in Table 1). It may take one ozone time scale (or 1–2.5 days) to "correct" the continuous ozone prediction in CMAQ after the meteorological fields are reset. Further analysis of the data is required to test for statistical significance and to determine the source of the relative change between day 1 and day 2. It is worth noting that the gain in skill in ozone prediction in day 2 is also shown using a smaller network of predominantly rural ozone observations in Part II but with a somewhat different trend through the MM5 run segment.

Figure 7 shows the rmse and its vector components for daily maximum 1-h ozone for each of the 35 days for NUDGE and NONUDGE. Willmott (1982) defines the mean-square-error (mse) as the sum of its systematic and unsystematic components, so it follows that rmse has a circular (or vector) relationship with rmses and rmseu. Willmott (1982) suggests that the systematic error should approach zero and the unsystematic error should approach the mse in a "good" model. Thus the rmse vectors shown in Fig. 7 are generally expected to be below the 1:1 line (which denotes rmses = rmseu).

As also indicated by Figs. 4a and 6a, Fig. 7 shows that rmse is generally lower for NUDGE than for NONUDGE. The 11 highest rmse totals (lowest skill days) during the 35-day period are in NONUDGE (shown by greatest distance from the origin in Fig. 7), while the 9 lowest rmse totals are in NUDGE. In addition, rmses overwhelms the rmseu for 6 of the 35 days in NONUDGE (indicating a lesser-skilled model), as shown by the data points above the 1:1 line in Fig. 7; rmses is not larger than rmseu on any of the days in the study period for NUDGE. Figure 7 also suggests that the skill in predicting daily maximum 1-h ozone tends to decrease with increased run time in MM5. The systematic component of the error tends to increase relative to the unsystematic component by day with respect to the MM5 run segment, as noted by the general counterclockwise shift of the rmse vector toward a higher systematic (and lower unsystematic) component of error. The trend toward a less skillful prediction of daily maximum 1-h rmse by partitioning of the components of rmse is seen in both NONUDGE and NUDGE. Figure 7 suggests that CMAQ predictions of daily maximum 1-h ozone tend to become less skillful, on average, as the MM5 run length increases, even when nudging is used in MM5 (i.e., in NUDGE) where there is no clear loss of skill in the near-surface meteorological variables in time. This is consistent with the aggregate by-day statistics shown in Fig. 4.

Table 2 shows the proportions of systematic and unsystematic error averaged by day within the MM5 run segment for NUDGE and NONUDGE. The systematic (SYS) and unsystematic (UNSYS) proportions are computed using the ratio of the (un)systematic mse to the total mse, defined by Willmott (1982). As in Fig. 7, there is a trend toward less skillful predictions of daily maximum 1-h ozone as illustrated with an increased proportion of systematic error as MM5 run length increases. This trend holds for both NONUDGE and NUDGE, although it is more subtle in NUDGE. In
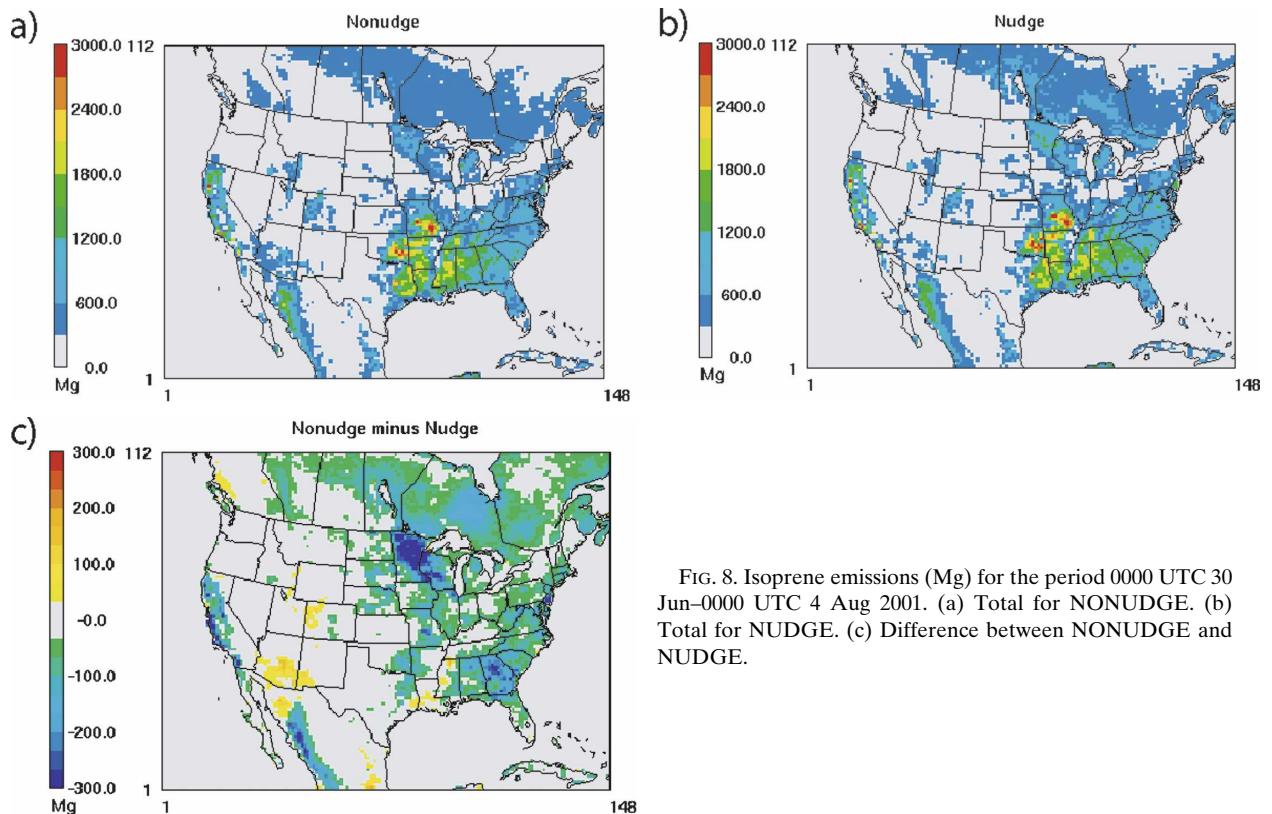
FIG. 8. Isoprene emissions (Mg) for the period 0000 UTC 30 Jun–0000 UTC 4 Aug 2001. (a) Total for NONUDGE. (b) Total for NUDGE. (c) Difference between NONUDGE and NUDGE.

addition, as in Figs. 4–7, there appears to be a gain in skill in day 2 when compared with day 1 in both NONUDGE and NUDGE.

An additional aspect of this work is to examine the impact of the changes in the meteorologically dependent emissions on the ozone predictions. As mentioned earlier, the biogenic and point-source sectors of the emissions are modulated by MM5. Figure 8 is a comparison of the total emissions of isoprene for NONUDGE and NUDGE for the 35-day analysis period. Isoprene, a biogenic ozone precursor, is typically emitted in forested locales and is a function of leaf temperature (i.e., 2-m temperature), solar radiation, and vegetation type (Pierce et al. 1998). Thus, the differences in isoprene emissions between NONUDGE and NUDGE are controlled solely by the changes to the MM5 simulations. Figures 8a and 8b show that the distribution of the isoprene emissions is spatially similar in NONUDGE and NUDGE, as expected, because the vegetation types are the same in both simulations. The magnitudes of the isoprene emissions are comparable, as the domainwide difference is 11% (not shown), and the local differences are typically less than 15% (Fig. 8c). Schwede et al. (2005), who modeled July 2001 (a large subset of the analysis period here) using the same geographical domain as used here, showed that a 44% domainwide reduction in isoprene emissions generally resulted in less than a 2-ppb difference in ozone predictions by CMAQ. The changes in emissions between NONUDGE and NUDGE are overall much smaller than in Schwede et al. (2005), so it is expected that the impact of the changes in biogenic emissions themselves on the ozone predictions is also small. In addition, the differences in the isoprene emissions increase as a function of MM5 run time (not shown), which largely reflects the divergent 2-m temperature fields between NONUDGE and NUDGE as MM5 simulation length increases (Figs. 1a), particularly during the daytime (Fig. 2a) when isoprene emissions are active. It is worth noting that the variability in the emissions estimates with or without nudging is small relative to the overall uncertainty in the emissions. A more comprehensive study would be required, however, to isolate the impacts of the meteorological fields from the emissions on the ozone predictions by CMAQ.

4. Discussion

This paper provides a demonstration of the impact of using nudging in the meteorological model on the retrospective air quality simulations using MM5 and CMAQ. A 35-day period is examined by binning the

MM5 and CMAQ simulation days according to time elapsed in each of the overlapping 5.5-day MM5 simulation segments. Evaluation of near-surface meteorological variables (2-m temperature, 2-m water vapor mixing ratio, 10-m wind speed, and 10-m wind direction) shows that, on average, there is no discernable degradation in skill in the MM5 dynamic analyses over the 5.5-day simulation period or at any point in the diurnal cycle. The MM5 simulation without nudging contains higher error, on average, with increased simulation duration when compared with the results obtained with dynamic analyses. The difference in average MAE between the dynamic analyses and the pseudoforecasts steadily increases from 0.23 K in day 1 to 0.84 K in day 5 for 2-m temperature, and it steadily increases from 0.25 to 0.53 m s^{-1} between days 1 and 5 for 10-m wind speed. Similar patterns for near-surface meteorological variables from day 1 to day 5 are seen in other simple statistical measures such as MBE, IA, and rmse when comparing the dynamic analyses with the pseudoforecasts. Within the diurnal cycle, the MAE averaged "by day" with time elapsed within the MM5 simulation shows a similar pattern on each of the 5 days used for CMAQ simulations for the dynamic analyses for near-surface meteorological fields. When nudging is not used in MM5, the error grows progressively with time elapsed, and it is exacerbated during the PBL growth period. The MM5 dynamic analyses that are used in this study are robust (no discernable loss of skill with increased simulation run time, on average), which suggests that 36-km dynamic analyses are reasonable for near-surface fields for at least 5.5-day simulations; an evaluation of the upper-air meteorological fields is warranted to determine whether the dynamic analyses are robust aloft, as well.

The initial results confirm that the CMAQ simulations that use dynamic analyses generated by MM5 with nudging compare more favorably to the daily maximum 1-h surface ozone observations than the CMAQ simulations that used MM5 pseudoforecast fields. The by-day-average rmse is lower for daily maximum 1-h ozone when the meteorological characterization is from the MM5 dynamic analyses as opposed to the forecasts, particularly from day 2 to day 5. For daily maximum 1-h ozone, widespread increases in rmse of 5 ppb from day 2 to day 5 are seen in the simulations where nudging is not used. There are more subtle but widespread decreases in statistical skill for daily maximum 1-h ozone in CMAQ as MM5 simulation run time increases when the MM5 dynamic analysis is used, as seen in by day averages of rmse, IA, and by the trend toward a greater proportion of systematic versus unsystematic rmse.

The statistical trend for daily maximum 1-h ozone, demonstrated by rmse and IA, does not mimic the trend for the meteorological state variables regardless of whether or not nudging is used in MM5. That is, the rmse and IA for daily maximum 1-h ozone in the CMAQ simulations with *and* without nudged meteorological fields show a marked improvement in skill in day 2 when compared with day 1, and a gradual decline in skill from day 2 to day 5. The trends in statistical skill are more pronounced in the CMAQ simulation that used the MM5 forecasts. The MM5 simulations do not gain skill in day 2 when compared with day 1. The MM5 dynamic analyses have fairly constant statistics through day 5, unlike the CMAQ simulations of daily maximum 1-h ozone that used those dynamic analyses that have increasing error with increased MM5 simulation length. The sources of the gain in skill in CMAQ in day 2 and the loss of skill as the MM5 simulation run time increases are unresolved at this time, but they may be related to physical discontinuities in the meteorological fields, the ozone time scale, and/or the accumulation of erroneous cloud cover in the meteorological model. Additional research is required to fully diagnose the cause of the change in skill in CMAQ as its run time relates to the MM5 run time.

The research presented in this paper affirms the use of nudging in the meteorological model to create dynamic analyses that provide the meteorological characterization for Eulerian chemical transport models. However, the behavior of the photochemistry is nonlinear, and its statistical skill does not directly parallel the statistical skill of the near-surface meteorological variables. Part II addresses evaluation against collocated meteorological and air quality measurements to gain insight into behavior of meteorological and photochemical fields at individual observation sites. Based on this work, additional research is recommended to optimize the method by which dynamic analyses are created for retrospective air quality modeling. For example, there is currently no research that suggests an optimal run length for meteorological dynamic analyses, and the use of overlapping 4–6-day periods has become somewhat of a de facto standard. The use of short-term, overlapping dynamical meteorological model simulations (e.g., 5.5-day MM5 run segments, as used herein) is largely an extension of using dynamic analyses for episodic air quality modeling (i.e., 4–6-day periods) and an artifact of the former constraint in MM5 that limited some ground-level fields (e.g., sea surface temperature, snow cover, soil temperature) to a static value throughout the duration of the run segment. Over the past several years, the land surface modeling techniques in MM5 and WRF have been vastly improved (e.g., Pleim and Xiu 2003), and the

focus in air quality modeling has shifted toward annual and multiyear simulations (e.g., Eder and Yu 2006; Gilliam et al. 2006; Hogrefe et al. 2006; Civerolo et al. 2007) to support multipollutant and climate-related issues. Seaman (2000) suggests that dynamic analyses could potentially be generated in continuous run segments of a year or more, although no research has demonstrated the utility of long run segments for air quality modeling applications. In addition, WRF is becoming a more mainstream model for air quality applications and there has been a stepwise move toward finer horizontal grid spacing for air quality modeling in the United States (e.g., Otte et al. 2005) concurrent with increases in computational capacity. Therefore, more attention should be given to the prescription of the meteorological input that is used for air quality models such as CMAQ for offline (one-way meteorological–air quality modeling) applications. Simulations of CMAQ with WRF-based input are suggested to determine if the trends found with MM5 fields are also found with WRF. Furthermore, the advances in variational data assimilation (e.g., Okamoto and Derber 2006) warrant exploration in concert with nudging for generating dynamic analyses for air quality modeling.

REFERENCES

Barna, M., and B. Lamb, 2000: Improving ozone modeling in regions of complex terrain using observational nudging in a prognostic meteorological model. *Atmos. Environ.,* **34,** 4889–4906.

Bey, I., and Coauthors, 2001: Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation. *J. Geophys. Res.,* **106,** 23 073–23 096.

Binkowski, F. S., and S. J. Roselle, 2003: Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component. 1. Model description. *J. Geophys. Res.,* **108,** 4183, doi:10.1029/2001JD001409.

Biswas, J., and S. T. Rao, 2001: Uncertainties in episodic ozone modeling stemming from uncertainties in meteorological fields. *J. Appl. Meteor.,* **40,** 117–136.

Black, T., 1994: The new NMC mesoscale Eta model: Description and forecast examples. *Wea. Forecasting,* **9,** 265–278.

Byun, D., and K. L. Schere, 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.,* **59,** 51–77.

Civerolo, K., and Coauthors, 2007: Estimating the effects of increased urbanization on surface meteorology and ozone concentrations in the New York City metropolitan region. *Atmos. Environ.,* **41,** 1803–1818.

Eder, B., and S. Yu, 2006: A performance evaluation of the 2004 release of Models-3 CMAQ. *Atmos. Environ.,* **40,** 4811–4824.

Environmental Protection Agency, 2003: User's guide to MOBILE6.1 and MOBILE6.2: Mobile source emission factor model. EPA Rep. EPA420-R-03-010, 262 pp. [Available online at http://www.epa.gov/otaq/models/mobile6/420r03010.pdf.]

Gilliam, R. C., K. W. Appel, and S. Phillips, 2005: The atmospheric model evaluation tool: Meteorology module. *Proc. Fourth Annual Models-3 Users' Conf.,* Chapel Hill, NC, Community Modeling and Analysis System, 6.1. [Available online at http://www.cmascenter.org/conference/2005/abstracts/6_1.pdf.]

——, C. Hogrefe, and S. T. Rao, 2006: New methods for evaluating meteorological models used in air quality applications. *Atmos. Environ.,* **40,** 5073–5086.

Grell, G. A., J. Dudhia, and D. R. Stauffer, 1994: A description of the fifth-generation Penn State/NCAR mesoscale model (MM5). NCAR Tech. Note NCAR/TN-398+STR, 138 pp.

Hogrefe, C., S. T. Rao, P. Kasibhatla, W. Hao, G. Sistla, R. Mathur, and J. McHenry, 2001: Evaluating the performance of regional-scale photochemical modeling systems. Part II—Ozone predictions. *Atmos. Environ.,* **35,** 4175–4188.

——, P. S. Porter, E. Gego, A. Gilliland, R. Gilliam, J. Swall, J. Irwin, and S. T. Rao, 2006: Temporal features in observed and simulated meteorology and air quality over the eastern United States. *Atmos. Environ.,* **40,** 5041–5055.

Houyoux, M. R., J. M. Vukovich, C. J. Coats Jr., N. M. Wheeler, and P. S. Kasibhatla, 2000: Emission inventory development

and processing for the Seasonal Model for Regional Air Quality (SMRAQ) project. *J. Geophys. Res.,* **105,** 9079–9090.

Kain, J. S., 2004: The Kain–Fritsch convective parameterization: An update. *J. Appl. Meteor.,* **43,** 170–181.

Mlawer, E. J., S. J. Taubman, P. D. Brown, M. J. Iacono, and S. A. Clough, 1997: Radiative transfer for inhomogeneous atmospheres: RRTM, a validated correlated-k model for the longwave. *J. Geophys. Res.,* **102,** 16 663–16 682.

Okamoto, K., and J. Derber, 2006: Assimilation of SSM/I radiances in the NCEP global data assimilation system. *Mon. Wea. Rev.,* **134,** 2612–2631.

Otte, T. L., 2008: The impact of nudging in the meteorological model for retrospective air quality simulations. Part II: Evaluating collocated meteorological and air quality observations. *J. Appl. Meteor. Climatol.,* **47,** 1868–1887.

——, A. Lacser, S. Dupont, and J. K. S. Ching, 2004: Implementation of an urban canopy parameterization in a mesoscale meteorological model. *J. Appl. Meteor.,* **43,** 1648–1665.

——, and Coauthors, 2005: Linking the Eta Model with the Community Multiscale Air Quality (CMAQ) modeling system to build a national air quality forecasting system. *Wea. Forecasting,* **20,** 367–384.

Pierce, T., C. Geron, L. Bender, R. Dennis, G. Tonnesen, and A. Guenther, 1998: Influence of increased isoprene emissions on regional ozone modeling. *J. Geophys. Res.,* **103,** 25 611–25 629.

Pleim, J. E., 2007: A combined local and nonlocal closure model for the atmospheric boundary layer. Part I: Model description and testing. *J. Appl. Meteor. Climatol.,* **46,** 1383–1395.

——, and J. S. Chang, 1992: A non-local closure model for vertical mixing in the convective boundary layer. *Atmos. Environ.,* **26A,** 965–981.

——, and A. Xiu, 2003: Development of a land surface model. Part II: Data assimilation. *J. Appl. Meteor.,* **42,** 1811–1822.

——, ——, P. L. Finkelstein, and T. L. Otte, 2001: A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. *Water Air Soil Pollut. Focus,* **1,** 243–252.

Rao, S. T., I. G. Zurbenko, R. Neagu, P. S. Porter, J. Y. Ku, and R. F. Henry, 1997: Space and time scales in ambient ozone data. *Bull. Amer. Meteor. Soc.,* **78,** 2153–2166.

Reisner, J., R. M. Rasmussen, and R. T. Bruintjes, 1998: Explicit forecasting of supercooled liquid water in winter storms using the MM5 mesoscale model. *Quart. J. Roy. Meteor. Soc.,* **124B,** 1071–1107.

Russell, A., and R. Dennis, 2000: NARSTO critical review of photochemical models and modeling. *Atmos. Environ.,* **34,** 2283–2324.

Sarwar, G., D. Luecken, G. Yarwood, G. Z. Whitten, and W. P. Carter, 2008: Impact of an updated carbon bond mechanism on predictions from the CMAQ modeling system: Preliminary assessment. *J. Appl. Meteor. Climatol.,* **47,** 3–14.

Schwede, D., G. Pouliot, and T. Pierce, 2005: Changes to the Biogenics Emissions Inventory System version 3 (BEIS3). *Proc. Fourth Annual Models-3 Users' Conf.,* Chapel Hill, NC, Community Modeling and Analysis System, 2.7. [Available online at http://www.cmascenter.org/conference/2005/abstracts/2_7.pdf.]

Seaman, N. L., 2000: Meteorological modeling for air-quality assessments. *Atmos. Environ.,* **34,** 2231–2259.

——, D. R. Stauffer, and A. M. Lario-Gibbs, 1995: A multiscale four-dimensional data assimilation system applied in the San Joaquin Valley during SARMAP. Part I: Modeling design and basic performance characteristics. *J. Appl. Meteor.,* **34,** 1739–1761.

Sistla, G., W. Hao, J.-Y. Ku, G. Kallos, K. Zhang, H. Mao, and S. T. Rao, 2001: An operational evaluation of two regional-scale ozone air quality modeling systems over the eastern United States. *Bull. Amer. Meteor. Soc.,* **82,** 945–964.

Stauffer, D. R., and N. L. Seaman, 1990: Use of four-dimensional data assimilation in a limited-area mesoscale model. Part I: Experiments with synoptic-scale data. *Mon. Wea. Rev.,* **118,** 1250–1277.

——, and ——, 1994: Multiscale four-dimensional data assimilation. *J. Appl. Meteor.,* **33,** 416–434.

——, ——, and F. S. Binkowski, 1991: Use of four-dimensional data assimilation in a limited-area mesoscale model. Part II: Effects of data assimilation within the planetary boundary layer. *Mon. Wea. Rev.,* **119,** 734–754.

——, ——, T. T. Warner, and A. M. Lario, 1993: Application of an atmospheric simulation model to diagnose air-pollution transport in the Grand Canyon region of Arizona. *Chem. Eng. Comm.,* **121,** 9–25.

Tanrikulu, S., D. R. Stauffer, N. L. Seaman, and A. J. Ranzieri, 2000: A field-coherence technique for meteorological field-program design for air quality studies. Part II: Evaluation in the San Joaquin Valley. *J. Appl. Meteor.,* **39,** 317–334.

Umeda, T., and P. T. Martien, 2002: Evaluation of a data assimilation technique for a mesoscale meteorological model used for air quality modeling. *J. Appl. Meteor.,* **41,** 12–29.

Willmott, C. J., 1982: Some comments on the evaluation of model performance. *Bull. Amer. Meteor. Soc.,* **63,** 1309–1313.

Xiu, A., and J. E. Pleim, 2001: Development of a land surface model. Part I: Application in a mesoscale meteorology model. *J. Appl. Meteor.,* **40,** 192–209.

Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the carbon bond chemical mechanism: CB05. Final report to the U.S. EPA, RT-0400675, 246 pp. [Available online at http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf.]