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Evaluating the performance of a computationally efficient MM5/CALMET system for developing wind field inputs to air quality models

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Abstract

The present study investigates the usefulness of coupling the prognostic MM5 mesoscale model with the CALMET diagnostic model for producing high resolution wind fields in a computationally efficient manner. Wind fields derived from this system are compared with the wind profiler observations from the Northeast-Oxidant and Particle Study (NE-OPS) field campaign over Philadelphia, PA undertaken during one of the summer ozone episodes in 1999 (23–24 July 1999). The MM5 simulations were performed on a nested grid (36, 12 and 4 km horizontal resolution) with 14 layers in the vertical direction for the period 21 July 1999; 00 UTC to 25 July 1999; 05 UTC. The CALMET meteorological model was applied with 14 layers in the vertical direction, a horizontal resolution of 4 km and a domain which includes New Jersey and the Philadelphia region and was employed in two modes. In the first mode, the MM5 model wind and mixing ratio output results (for 36, 12 and 4 km horizontal resolution) are ingested every hour into the CALMET diagnostic meteorological model along with an objective analysis procedure using all available observations. In the second mode, no MM5 results were utilized and CALMET employed the objective analysis procedure. All the above simulations are compared with the wind profiler data collected during the NE-OPS program. The results of this study indicate that utilizing the coarsest prognostic meteorological model output in a diagnostic model provides an attractive option for generating accurate meteorological inputs for air quality modeling studies, especially for long-term simulations of periods lasting from several weeks to a year. While the mean relative errors for the meridional component of velocity decreased significantly when the CALMET model was operated in the first mode, there was no corresponding significant decrease in the relative errors for the zonal component of velocity in the above mode.

Keywords: CALMET; Diagnostic; MM5; Profiler; NARSTO; NE-OPS

1. Introduction

1.1. Rationale

Three-dimensional photochemical grid models are increasingly being used by state and federal agencies for developing emission control strategies to improve air quality. Presently, there is a critical need to perform long

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term (i.e. annual) regional photochemical air quality simulations. In response to this need the US Environmental Protection Agency (EPA) carried out meteorological and air quality simulations over the Ozone Transport Assessment Group (OTAG) domain (Eastern US) for the entire year of 1995. The Fifth Generation Penn State/NCAR Mesoscale Model (MM5) (Grell et al., 1994) and the Community Multiscale Air Quality (CMAQ) model were utilized by the US EPA to carry out air quality modeling studies over this domain using a coarse 36 km horizontal resolution. It would of course be computationally prohibitive to pursue a similar effort as undertaken by US EPA with much finer horizontal resolution, such as 4 km. The need for the higher resolutions is, nevertheless, critical for various air quality and human exposure studies, e.g. those focusing on densely populated urban areas in the NE corridor. One possibility is to perform long-term high resolution CMAQ (or other) simulations on a local grid, utilizing the outputs of the coarse grid CMAQ simulations as inputs. The present study explores the possibility of utilizing (ingesting) the 36 km MM5 winds over the OTAG domain to a finer resolution diagnostic model such as the California Meteorological model/photochemical model (CALMET) on a domain centered over the respective focus study area (in this case the New Jersey and Metropolitan Philadelphia region). The meteorological output from CALMET after ingesting the 36 km MM5 wind output can then be utilized in photochemical models such as CMAQ to provide for accurate air quality simulations for the individual state or local areas. This approach can provide accurate meteorological inputs (by combining prognostic meteorological model output with actual observations via the diagnostic model), thus allowing the state agencies to formulate the necessary emission control strategies for their respective states or non-attainment regions.

1.2. Background

The basic approach for constructing the meteorological fields typically utilizes either a prognostic model or a diagnostic model. Diagnostic models (Sherman, 1978; Goodin et al., 1980; Douglas and Kessler, 1988; Scire et al., 2000) take into account by the available observations, topography of terrain as well as constraints such as conservation of mass (Pielke and Uliasz, 1998). Since the diagnostic models interpolate observational data, they are critically dependent on the quality and the density of these observations. Despite their limitations, diagnostic models have been used extensively in air quality modeling studies. Prognostic meteorological models (in which primitive equations that govern the state of the atmosphere are solved), are being increasingly used to provide the meteorological inputs for air quality modeling studies (Pielke and Uliasz, 1998; Sistla et al., 1996). However, the problem of the full prognostic model is a formidable one and uncertainties in inputs as well as simplifying assumptions in the prognostic model formulations can cause predictions which do not match actual observations. It is of course possible to incorporate observations into prognostic models through analysis/observational nudging, to improve the prediction of the certain variables. Also, the computational costs and required computer time needed to run the prognostic models are still high. One solution is to use a combination of both prognostic and diagnostic models, thereby complementing their individual advantages. The computational costs involved in running a coarse prognostic meteorological model and ingesting its output to a fine resolution diagnostic model simulation, are significantly lower than running a fully nested prognostic meteorological model with horizontal resolutions comparable to those of the diagnostic model. Ultimately the success of the coupled prognostic/diagnostic modeling approach would lie in its evaluation with actual observations.

Alapaty et al. (1995) investigated the sensitivity of the US EPA Regional Oxidant Model (ROM) to differing meteorological (prognostic MM4 and diagnostic model) inputs over the eastern US. The comparisons of predicted concentrations of chemical species indicated higher values (1–5 ppb for NO_x and 1–25 ppb for reactive organic gases) when the prognostic model outputs were used. Kumar and Russell (1996) investigated the impact of prognostic (MM4) and diagnostic meteorological inputs on photochemical air quality modeling performance for the Southern California region during the Southern California Air Quality Study (SCAQS) period (27–29 August 1987). The results indicated that the temperature and mixing heights derived from the prognostic models agreed better with observations as compared to velocity data. However, the results obtained from the photochemical models were similar for both inputs except that a lower ozone peak was predicted using the prognostic meteorological inputs. Eastman et al. (1995) compared model simulations with tracer data for the western shore of Lake Michigan, utilizing the EPA regulatory Industrial Source Complex Short Term (ISCST) model and the Lagrangian Particle Dispersion Model (LPDM). The results of the study indicated clearly that the observed tracer data were consistent with the simulated tracer behavior obtained from the prognostic LPDM model while the agreement with the diagnostic model was not consistent. Barna et al. (2000) ventured to utilize the MM5 output as an initial guess wind field for CALMET to create the meteorological fields for July 1996 in the Cascadia region. The predicted ozone concentration by the California Grid Model (CALGRID) agreed well with observations at the monitors located along the Interstate Highway No. 5 corridor. Barna and Lamb

(2000) also carried out three air quality simulations using CALGRID for an ozone episode which occurred in the Cascadia region of the Pacific Northwest during 11–14 July 1996. The above three air quality simulations individually utilized the wind field obtained from the MM5 model without observational nudging, MM5 model output without observational nudging as an initial-guess field for CALMET, and finally the MM5 model output with observational nudging. The results indicated that ozone predictions significantly improved when the MM5 output with observational nudging was used, compared with the other two simulations. Hanna et al. (1996) evaluated various photochemical grid models such as the Urban Airshed Model with Variable Grid (UAM-V), the EPA regulatory version of the Urban Airshed Model Carbon Bond IV (UAM-IV) and the UAM-IV nested with the Regional Oxidant Model (UAM-IV/ROM), with data obtained from two 3-day ozone episodes during the 1991 Lake Michigan Ozone Study (LMOS). While all the above photochemical models utilized the meteorological input from the diagnostic model CALMET, an additional simulation of UAM-V utilizing meteorology obtained from a prognostic model (CALRAMS) was undertaken. The results of the study indicated that there was little effect on the UAM-V performance statistics from using a diagnostic or prognostic meteorology, except that the spatial location of the broad regional ozone plume was better simulated when the prognostic meteorological model was used. Recently, Mass et al. (2002) studied the effects of increasing horizontal resolution on the forecast skill by examining the results of two years of the University of Washington Real-Time MM5 Modeling and Verification System over the Pacific Northwest and found that decreasing grid spacing does improve the realism of the results but does not necessarily improve significantly the skill accuracy of the forecasts. Fast et al. (2002) studied the relative role of local and regional scale processes on ozone in Philadelphia for the period 15 July–4 August 1999 by utilizing a coupled meteorological and chemical modeling system, PNNL Eulerian Gas and Aerosols Scalability Unified System (PEGASUS). The results indicated little model bias in the simulated wind speed as compared to the wind profilers but the simulated wind directions were more westerly by about 15°.

1.3. A brief overview of NARSTO-NE-OPS

The North American Research Strategy for Tropospheric Ozone-Northeast-Oxidant and Particle Study (NARSTO-NE-OPS) is a multi-institutional collaborative research program set up under an EPA initiative to improve current understanding of the underlying causes for the occurrence of high ozone concentrations and increased levels of fine particles in the Northeastern United States. Various advanced meteorological (aircraft, lidar, tethered balloon and radar wind profiler/radio acoustic sounding system (RASS) sounder) and air chemistry (ground based particle/chemical samples) measurements were made at the Baxter Water Treatment Plant, Philadelphia, PA (40.0764° N, 75.0119° W) during three field campaigns conducted during the summers of 1998, 1999 and 2001 (Philbrick et al., 2002). The Pennsylvania State University Radar wind profiler/RASS sounder were operated at the Baxter Water Treatment Plant site during the NE-OPS campaign. The present investigation was primarily focused on an ozone episode that took place on 23–24 July 1999 over the Philadelphia region and the horizontal wind components obtained from the CALMET model were compared with the NE-OPS profiler data at the Baxter site. Since the tethered balloon data were confined to within 300 meters, the comparison with the NE-OPS observations is restricted to the wind profiler only.

2. Meteorological modeling: approach

2.1. Prognostic meteorological model: MM5

The meteorological model utilized in the present study is the MM5 Model Version 3.4. Fourteen layers in the vertical direction (centered at $\sigma = 0.9975$, 0.9925, 0.985, 0.9725, 0.955, 0.9325, 0.9, 0.84, 0.75, 0.65, 0.525, 0.375, 0.225 and 0.075) and three levels of one-way nested domains were used with grid resolutions of 36, 12 and 4 km. The outermost domain encompasses the entire eastern United States while the inner domain just encompassed the Philadelphia and New Jersey region. The number of grid cells in the east–west and north–south directions are 75×69, 52×52 and 67×76 at the 36, 12 and 4 km resolutions, respectively. The study utilized the Blackadar scheme for planetary boundary layer (PBL), the Grell scheme for cumulus parameterization (for 36 and 12 km domains only), a mixed phase (Reisner) scheme for explicit moisture, a cloud radiation scheme and a force restore (Blackadar) scheme for ground temperature. In addition to surface and rawinsonde observations, the ECMWF global analysis data at 2.5° resolution were utilized. Four dimensional data assimilation (FDDA) option through analysis nudging was utilized in the free atmosphere to nudge horizontal winds, temperature and moisture for all domains. In the PBL, the winds were nudged using the surface data through analysis nudging while temperature and moisture were not nudged within the PBL. Model simulations were performed for the period between 21 July 1999; 00 UTC and 25 July 1999; 05 UTC. The output frequency of the MM5 model was set to 1 h and the pressure at the model top for MM5 was set at 100 hPa.

2.2. Diagnostic meteorological model: CALMET

The CALMET model incorporates an advanced version of the Diagnostic Wind Model (DWM) (Douglas and Kessler, 1988) and produces mixing height fields and other meteorological parameters that are typically utilized by the Langranian puff dispersion model CALPUFF, or the Eulerian photochemical transport model CALGRID, or the Lagrangian Kinematic Simulation Particle (KSP) model. The wind field outputs from the 36, 12 and 4 km MM5 model were ingested into the CALMET model as an initial-guess wind field. In this case, the prognostic winds are interpolated to the fine-scale CALMET grid and the normal diagnostic adjustments for the fine-scale terrain are made. Finally, an objective analysis procedure is employed using all available observations. In addition to the following default output variables (pressure, elevation, temperature, wind speed and wind direction), the user can request a maximum of five sets of additional variables such as vertical velocity, relative humidity/vapor mixing ratio, cloud and rain mixing ratio, ice and snow mixing ratio and graupel mixing ratio to be output from MM5. In this study all the additional variables except the graupel mixing ratio were output from MM5. However, CALMET does not use other important parameters such as mixing height, cloud cover etc. from MM5 and hence calculates its own mixing heights. The CALMET model utilized 14 layers in the vertical direction with the layers being centered at ($z = 10$, 50, 115, 187.5, 262.5, 425, 712.5, 1075, 1730, 2892.5, 4187.5, 5387.5, 6800 and 8300 m), where z is the terrain following vertical coordinate system. The CALMET domain is centered around the New Jersey and Metropolitan Philadelphia region with a grid of 75×75 cells in each layer and a horizontal resolution of 4 km (Fig. 1). The CALMET model utilized routine NWS observations with upper air rawinsonde data (available every 12 h) from seven stations and hourly surface data from thirty surface stations and one overwater station. The CALMET simulations were performed for the period between 21 July 1999; 00 UTC and 25 July 1999; 05 UTC. In addition to the above simulations, the CALMET model was also utilized in a second mode wherein CALMET uses the one upper air sounding inside the domain as an initial guess wind field, applies the normal diagnostic adjustments for terrain and employs the objective analysis procedure using all available observations. No MM5 data were utilized in this second CALMET mode. The CALMET simulations in both modes were evaluated with the NE-OPS wind profiler observations over Philadelphia. It is pertinent to note that the above NE-OPS wind profiler observations were not utilized in either the FDDA used in MM5 or in the analysis procedure used in CALMET, and hence an evaluation of the CALMET simulations in both modes with the NE-OPS wind profiler observations is indeed meaningful.

3. Results and discussion

The prognostic 36, 12 and 4 km MM5 wind and mixing ratio outputs were ingested individually to CALMET as an initial-guess field and the normal diagnostic adjustments for fine-scale terrain were performed. CALMET, in addition to the above initial-guess field from MM5, also utilized the surface, overwater and upper air observations to obtain accurate meteorological wind fields. In order to investigate the effect of MM5 ingestion, another simulation (CALMET in the second mode) was undertaken without any MM5 ingestion and all four simulations were compared with the NE-OPS wind profiler observations. The NE-OPS wind profiler observations were available for 22 vertical levels up to 22 July 1999; 16 UTC and for 35 vertical levels thereafter. The horizontal wind vector NE-OPS observations with 22 vertical levels are shown in Fig. 2a for the period 21 July 1999; 00 UTC to 22 July 1999; 16 UTC. Figs. 2b–3c depict the horizontal wind vectors from CALMET simulations in the second mode (Fig. 2b) and the CALMET simulations in the first mode (using wind and mixing ratio outputs from 36, 12 and 4 km MM5 simulations). The cold front which terminated the strong ozone episode of 16–19 July 1999 over Northeast US finally drifted south of the region early on 21 July 1999 (Ryan, 2000). However, the front had begun to move slowly north by early morning of 22 July 1999. Although winds aloft were steady northwesterly throughout the day on 22 July 1999, the local wind fields were quite complex with low level winds changing to southerly as the remnants of the stationary front drifted northward (Ryan, 2000). It is clear that the CALMET simulations in the first mode (Figs. 3a–c) are closer to observations (Fig. 2a) than CALMET simulations in the second mode (Fig. 2b). While the CALMET simulations in the first mode successfully reproduce the observed change in the wind direction (from southwesterly at 1700 m to northwesterly at above 3000 m), the CALMET simulations in the second mode fail to reproduce the above vertical structure. The above may be due to the fact that only one upper air station, in Brookhaven, NY, is located within the CALMET domain and this station is a distance from Philadelphia (approximately 194 km). However, the CALMET simulations in both modes do successfully simulate the low level southerlies seen in Fig. 2a. There are some instances of improved CALMET simulations in the first mode when using 12 and 4 km MM5 results over CALMET simulations which use 36 km MM5 results. While the CALMET simulations using 36 km MM5 results depict an incorrect

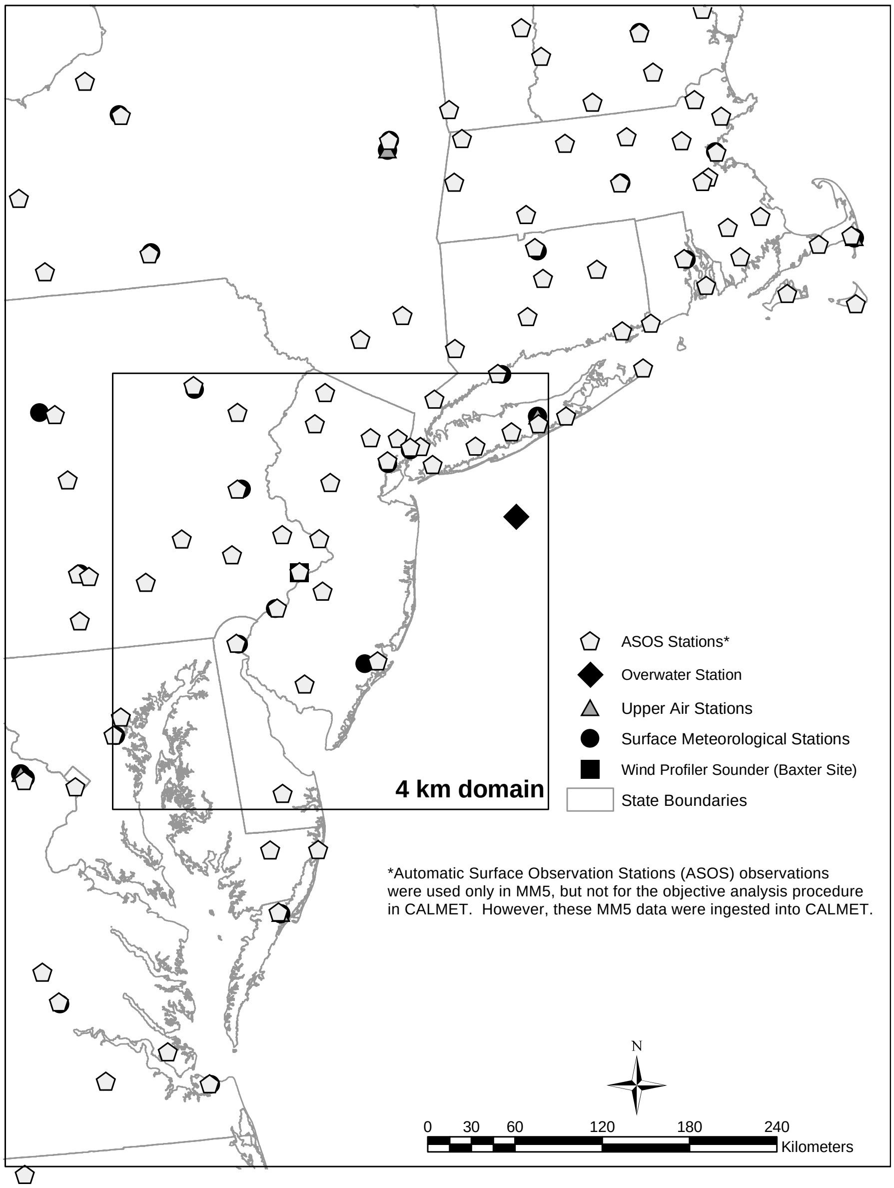

Fig. 1. The CALMET modeling domain with 4 km horizontal grid resolution. The projection shown above is Lambert Conformal, with the first and second parallels being 30° and 60° and the reference longitude and latitude being 84.36° W and 37.34° N.

southwesterly in the lower levels on 21 July 1999; 12 UTC (Fig. 3a), the CALMET simulations using 12 and 4 km MM5 simulations reproduce the correct southerly flow (Figs. 3b and c) as seen in the observations.

Fig. 4a depicts the horizontal wind vector NE-OPS observations with 35 levels in the vertical direction for the period 22 July 1999; 17 UTC to 25 July 1999; 05 UTC. The low level winds changed from southerly to drier westerly flow by 21 UTC on 22 July 1999. However, by morning of 23 July 1999 the upper air ridge had moved east and the winds returned to the north appearing as northeast at low levels and strong northerly aloft (Ryan, 2000). Winds again reverted at low levels to southwesterly late in the afternoon of 23 July 1999 while steady southwesterlies are seen at all levels on 24 July 1999 from 12 UTC throughout the night (Ryan, 2000). Figs. 4b–d depict the horizontal wind vectors from CALMET simulations in the second mode and in the first mode for the same period as depicted in Fig. 4a. The CALMET simulation in the first mode using 4 km MM5 simulation for the above mentioned time period is not included for brevity as it

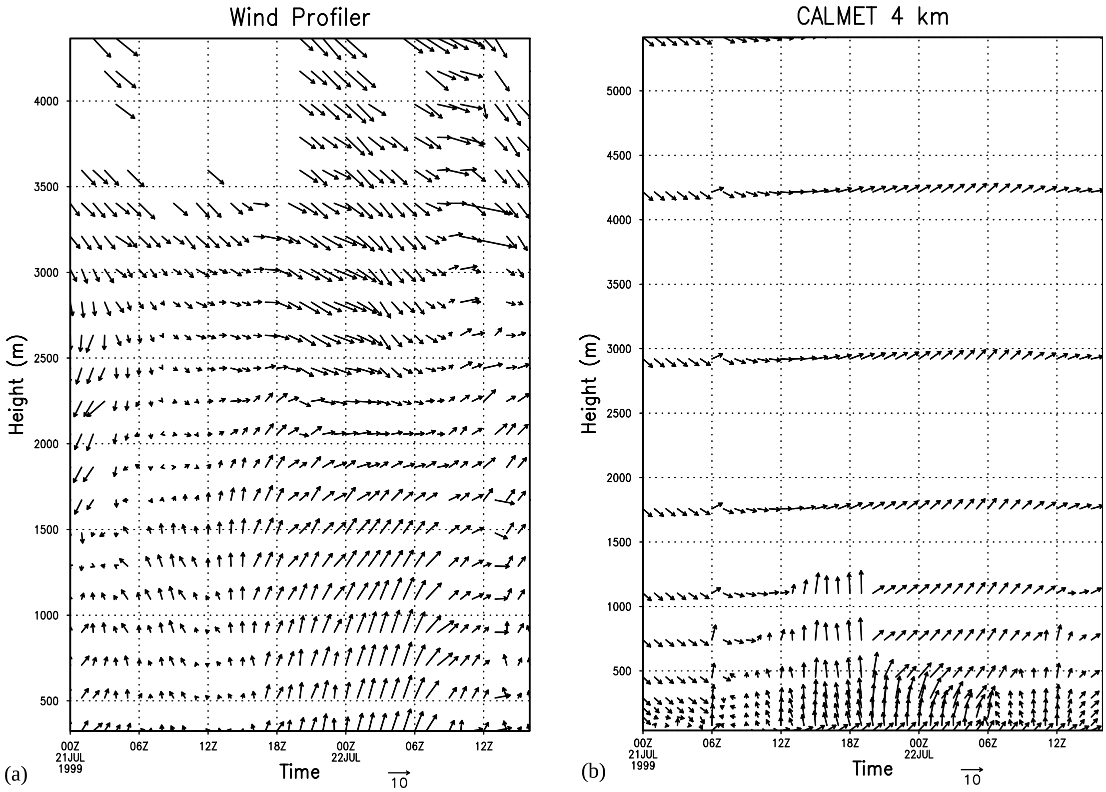

Fig. 2. Horizontal wind vector field for the period 21 July 1999; 00 UTC to 22 July 1999; 16 UTC. (a) NE-OPS wind profiler observations and (b) CALMET simulations in the second mode.

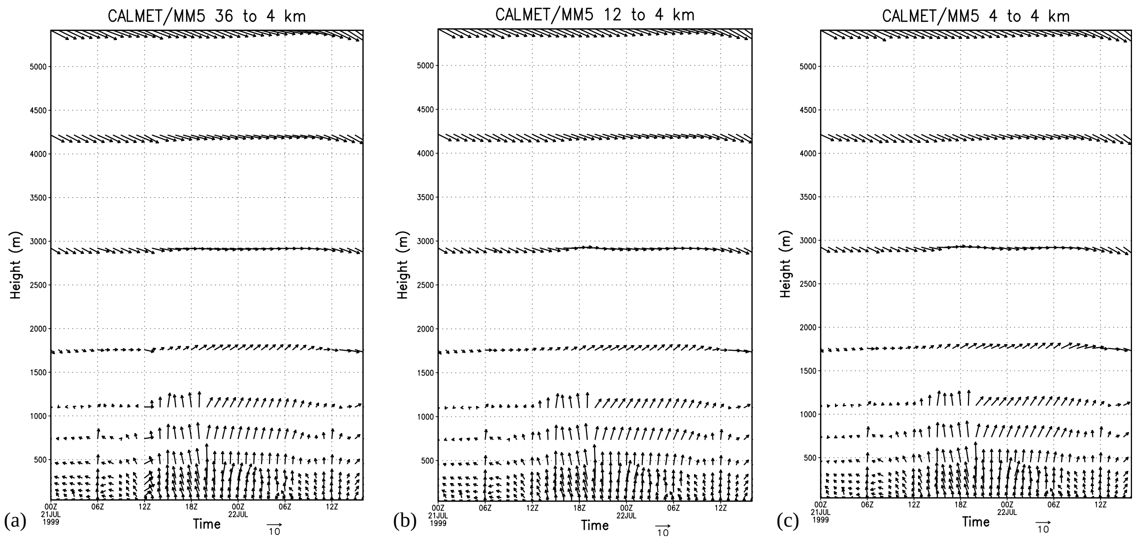

Fig. 3. Horizontal wind vector field for the period 21 July 1999; 00 UTC to 22 July 1999; 16 UTC. CALMET simulations in the first mode using (a) 36 km MM5, (b) 12 km MM5 and (c) 4 km MM5.

is quite similar to Fig. 4d. The strong northerlies seen aloft during the morning hours of 23 July 1999 appear as northwesterlies in Figs. 4c and d (CALMET simulations in the first mode) and as weak northwesterlies in Fig. 4b (CALMET simulations without MM5). The CALMET simulation in the second mode produces weaker winds

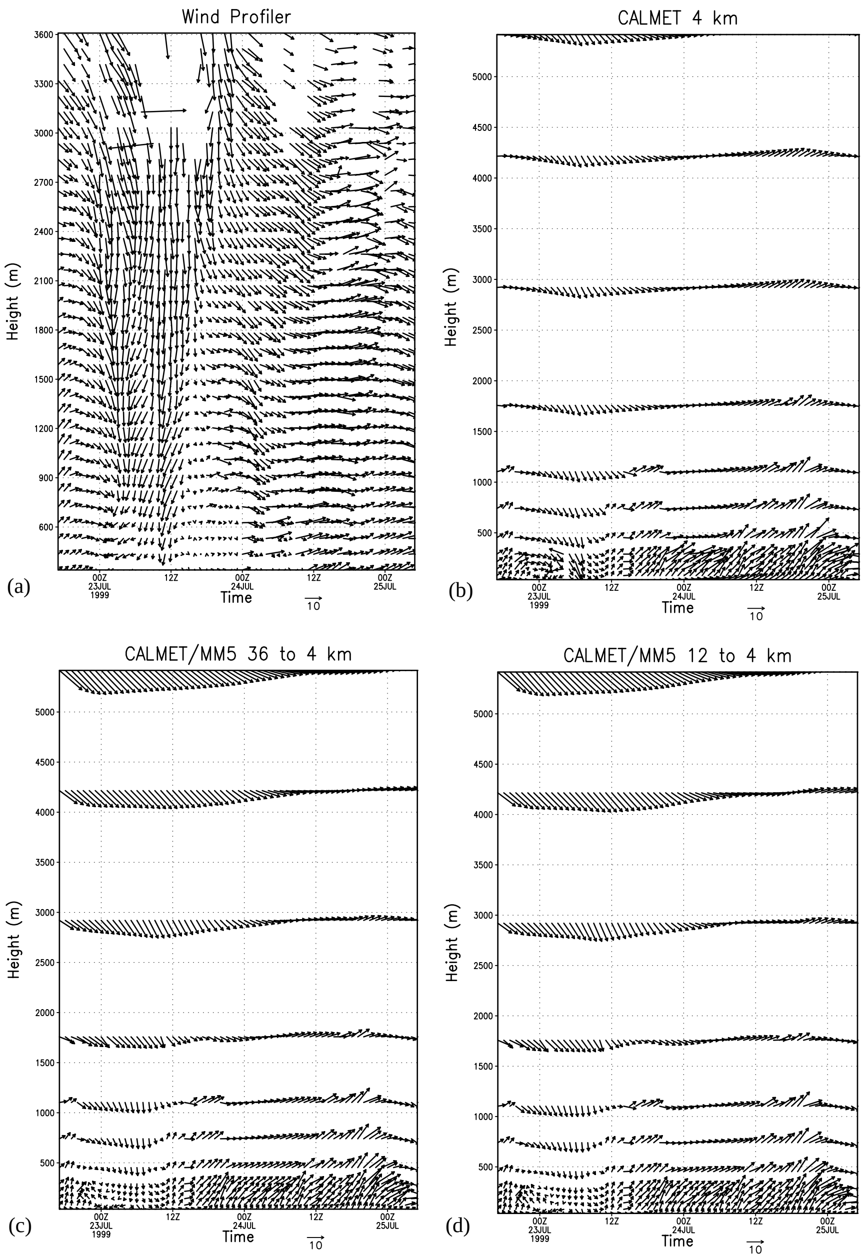

Fig. 4. Horizontal wind vector field for the period 22 July 1999; 17 UTC to 25 July 1999; 05 UTC. (a) NE-OPS wind profiler observations, (b) CALMET simulations in the second mode. CALMET simulations in the first mode using (c) 36 km MM5 and (d) 12 km MM5.

aloft due to inadequate density of upper air stations within the CALMET domain. The CALMET simulations in the second mode appear to predict the low level winds (at 200 m) better than CALMET simulations in the first mode for the period 22 July 1999; 20 UTC to 23 July 1999; 01 UTC. The above may be attributed to the fact that the MM5 simulations (including 4 km) are not fine enough to fully resolve the observed terrain-induced features of the flow. The near calm conditions observed on 23 July 1999 between 12 UTC and 23 UTC are not reproduced by the CALMET simulations in either mode.

Figs. 5a–d depict the mean relative error of the zonal component of the velocity over the observational vertical levels for the CALMET simulations in the second mode (Fig. 5a) and for the first mode (using 36,

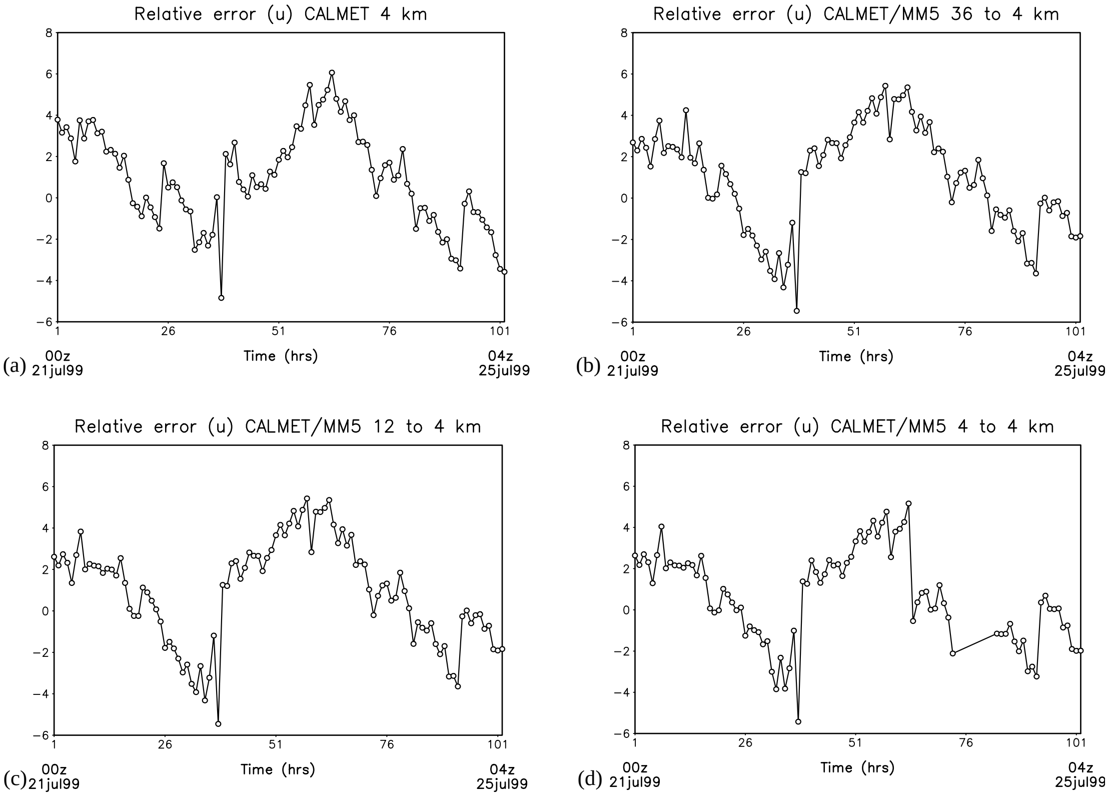

Fig. 5. Mean relative error of zonal component of velocity over all observational vertical levels for the period 21 July 1999; 00 UTC to 25 July 1999; 04 UTC. (a) CALMET simulations in the second mode; (b)–(d) CALMET simulations in the first mode using (b) 36 km MM5, (c) 12 km MM5 and (d) 4 km MM5.

12 and 4 km MM5 simulation) for the period 21 July 1999; 00 UTC to 25 July 1999; 04 UTC. Figs. 6a–d depict the mean relative error of the meridional component of velocity for the above mentioned time period. While the CALMET simulations in the first mode (with MM5) revealed significant improvements for the meridional components compared to the CALMET simulations in the second mode, no such improvements were noticed for the zonal component of the velocity. The percentage of times when the mean relative error for the meridional component of velocity had a magnitude less than 1 m s^{-1} rose from 18% for CALMET simulations in the second mode to 33% for CALMET simulations using 4 km MM5. The corresponding figures for CALMET simulations using 36 km MM5 outputs and 12 km MM5 outputs were 30% and 31%, respectively. Also, the percentage of times when the mean relative error for the meridional component of velocity had a magnitude of more than 2 m s^{-1} fell from 62% for CALMET simulations where no MM5 outputs were utilized to 38% for CALMET simulations using 4 km MM5 outputs. The corresponding figures for CALMET simulations using 36 km MM5 and 12 km MM5 outputs were 45% and 44%, respectively. However, the percentage of times when the mean relative error for the zonal component of velocity had a magnitude of more than 2 m s^{-1} was 47% for both CALMET simulations using 4 km MM5 outputs and for CALMET simulations in the second mode. The inability of the CALMET simulations in the second mode to reproduce the change in wind direction aloft from southwesterly to northwesterly for the period between 21 July 1999; 18 UTC and 22 July 1999; 16 UTC, and the weakened northerlies simulated aloft by the CALMET simulations in the second mode for the period 23 July 1999; 00 to 12 UTC, would both contribute to larger mean relative error for the meridional component of velocity.

The largest mean relative error for the zonal component of velocity occurs at $t = 38$ (22 July 1999; 13 UTC) (Figs. 5a–d). The wind profiler observations prior to this hour up to a height of 1600 m are southwesterly and change to westerly at 13 UTC and yet again abruptly to southerlies at the next hour (Fig. 2a). There is a possibility that the above mentioned large relative error for the zonal component could be attributed to the observations themselves. The largest mean relative error for the meridional component of velocity occurs at $t = 60$ (23 July 1999; 11 UTC). The

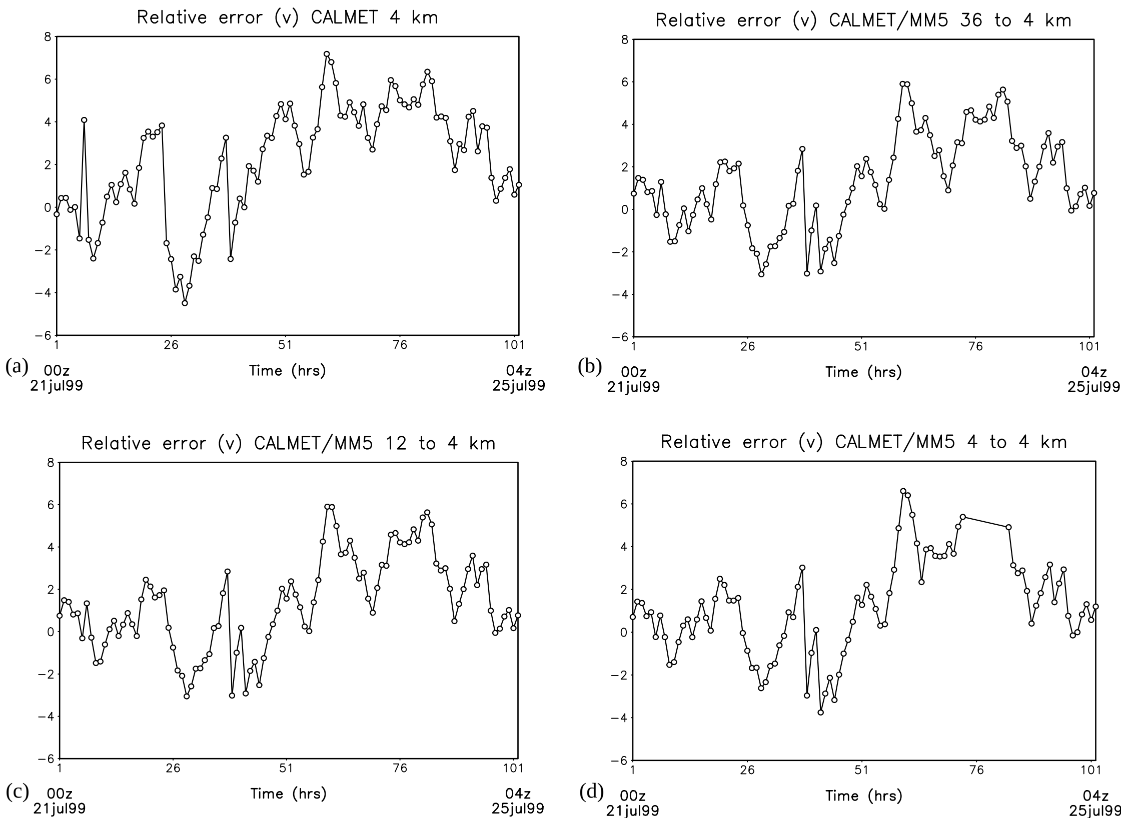

Fig. 6. Mean relative error of meridional component of velocity over all observational vertical levels for the period 21 July 1999; 00 UTC to 25 July 1999; 04 UTC. (a) CALMET simulations in the second mode; (b)–(d) CALMET simulations in the first mode using (b) 36 km MM5, (c) 12 km MM5 and (d) 4 km MM5.

above time coincides with the occurrence of the strongest northerlies aloft. The CALMET simulations in the second mode for the above time predict weak northwesterlies while the CALMET simulations in the first mode predict moderate northwesterlies. It is evident from Figs. 2a and 4a that the meridional component of velocity exhibits more frequent reversal of signs than the zonal component of velocity. The CALMET simulations in the first mode, which utilizes the prognostic MM5 winds, possibly do a better job of reproducing the observed changes in the meridional component of velocity and hence perform better than the CALMET simulations in the second mode. However, for the zonal component of velocity, with less marked changes in sign, the efficacy of the CALMET simulations in the first mode may be lower.

4. Conclusions

This study investigated the feasibility and usefulness of ingesting the prognostic meteorological (MM5 wind and mixing ratio) output to a diagnostic meteorological model (CALMET) to obtain a more accurate meteorological wind field for air quality modeling studies. All four CALMET simulations (ingesting 36, 12 and 4 km MM5 output and no MM5 ingestion) were compared to one another and also with the wind profiler observations from the NE-OPS field campaign at Philadelphia during a summer ozone episode (23–24 July 1999). The results of the study indicate that the CALMET predictions with MM5 ingestion are much closer to observations as compared to the case without any ingestion. There are very small differences in the horizontal wind components between the CALMET predictions for the case of MM5 ingestion outputs at three horizontal resolutions. The above results indicate that utilizing the coarsest prognostic meteorological model output as input for a diagnostic model provides an attractive option for generating accurate meteorological inputs for air quality modeling studies, especially for long-term simulations, i.e. periods lasting from several weeks to a year. While it is true that the above results may generally hold for a region of relatively simple terrain, regions of complex terrains can introduce additional difficulties like inadequate density of observations, limitations of a diagnostic model to reproduce the observed features over complex terrain, and difficulties in fully resolving terrain features by using a coarse prognostic model over a complex terrain. The effectiveness of this approach may therefore be different for a region of complex terrain.

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