J7.13

# A COMPARATIVE STUDY OF PROGNOSTIC METEOROLOGICAL AND OF AIR QUALITY MODEL PREDICTIONS WITH NEOPS 1999 OBSERVATIONS

**A. Chandrasekar, Q. Sun and P.G. Georgopoulos**
Environmental and Occupational Health Sciences Institute (EOHSI), Piscataway, New Jersey 08855

**Abstract** This study presents a comparative evaluation of prognostic mesoscale meteorological and of photochemical gas/aerosol air quality model predictions with data from the North East Oxidant and Particle Study (NE-OPS) research program over Philadelphia, PA. Model simulations were performed for a two week period from 11th July 1999 00 UTC to 25th July 1999 11 UTC corresponding to the field study days for NEOPS. The MM5 model was applied with 14 layers in the vertical direction and the results were compared with aircraft, RASS, wind profiler, lidar and tethersonde balloon data collected by the NE-OPS program. Comparisons with aircraft data indicate that while the MM5 model successfully reproduces the observed temperature values, this is not the case with relative humidity values. The virtual temperature profiles predicted by the model compare very well with RASS data while the wind components calculated by the model are only in partial agreement with the wind profiler data. However the mixing ratio and temperature profiles obtained from lidar compare well with the model results. The model predicted meteorological variables are only in partial agreement with the tethersonde balloon observations with both relative humidity and wind speed being underestimated by the model. US EPA's Community Multiscale Air Quality (CMAQ) model, a component of the Models-3 system, and MCNC's Multiscale Air Quality Simulation Platform (MAQSIP) were used to simulate gaseous and aerosol phase air quality dynamics for the same domain. The modal aerosol model included as part of the current release of CMAQ is used in the CMAQ simulations while the dynamic sectional aerosol developed at the University of Delaware (UDAERO) is adopted in the MAQSIP simulations. The emissions data were processed from the National Emissions Trends (NET) inventory using MCNC's Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. Fourteen layers in the vertical direction and three levels of nested domains are used, with grid resolution of 36 km for the outermost domain, 12 km for the intermediate domain and 4 km for the innermost domain encompassing the metropolitan Philadelphia area. The model predictions were compared with chemically and temporally resolved pollutant concentration measurements obtained through the NEOPS study to evaluate the performance of the models in capturing the 3-dimensional regional scale dynamics of ozone and particulate matter.

## 1. INTRODUCTION

The North American Research Strategy for Tropospheric Ozone – North East Oxidant and Particle Study (NARSTO-NE-OPS) is a multi institutional collaborative research program set up to improve current understanding of the underlying causes for the occurrence of high ozone concentrations and increased levels of fine particles in the north-eastern United States. Various advanced meteorological and air chemistry measurements were made in the vicinity of Philadelphia, Pennsylvania during two field campaigns conducted during the summer of 1998 and 1999 (Philbrick et al, 2000). The University of Maryland provided information on the distribution of particulate matter, chemical species and meteorology by operating the instrumented flights with Cessna and Aztec aircrafts over Philadelphia airport (PNE) and Tipton Airport, Ft. Meade, MD (FME)(Doddridge 2000). Radar wind profiler/RASS sounder were operated at the Baxter (Philadelphia Air Management) and West Chester (Pacific Northwest National Laboratory, PNNL) sites while a radar wind profiler was stationed at the Pittsgrove site (Argonne National Laboratory, ANL). The Pennsylvania State University Lidar, referred to as LAPS (Lidar Atmospheric Profile Sensor), developed as a prototype for the U.S. Navy, was utilized to obtain vertical profiles of ozone, water vapor, temperature and extinction during the summers of 1998 and 1999 at the Baxter site. The LAPS instrument uses multi-channel photon counting detection to measure several wavelengths of Raman scattered signals which ultimately yields vertical profiles of atmospheric properties (Mulik et al. 2000). Millersville University deployed two tethersonde balloons during the summers of 1998 and 1999 to obtain detailed temporal and vertical profiles of fine particles, $O_3$ concentrations and meteorological variables (Clark 2000). In addition to the above, aircraft measurements (Brookhaven National Laboratory), ozonesondes (PNNL), rawinsondes (PNNL, ANL) and ground based measurements of particle/chemical samples (Harvard University School of Public Health) were conducted. The meteorological data provided by the University of Maryland instrumented aircraft were restricted to temperature and relative humidity at different pressure and altitude levels in the atmosphere. The radar wind profiler provided the profiles for all three velocity components while the RASS (Radio Acoustic Sounding System) sounder provided profiles of the virtual temperature and vertical velocity respectively. The tethersonde balloons provided profiles of dry and wet bulb temperature, atmospheric pressure, wind speed and direction, and $O_3$ concentration while the meteorological data provided by Lidar were restricted to temperature and mixing ratio profiles. The present investigation was primarily focused on a major ozone episode that took place in July 1999 over the Philadelphia region, to perform an extensive evaluation of the MM5 (Grell et al., 1994) and CMAQ (Byun and Ching, 1999).

## 2. PROGNOSTIC METEOROLOGICAL MODELING

The meteorological model utilized in the present study is the Fifth Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) (Grell et al. 1994). 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, 0.075) and three levels of nested domains were used with grid resolutions of 36 km for the outermost domains, 12 km for the intermediate domain and 4 km for the innermost domain. The outermost domain encompasses the entire eastern United States while the inner domain encompasses the Philadelphia and New Jersey region (Figure 1). The grid dimensions in the east-west and north-south directions are 75 x 69, 52 x 52 and 67 x 76 at the 36, 12 and 4 km resolutions, respectively. The study utilized the high resolution Blackadar scheme for Planetary Boundary Layer (PBL), the Grell scheme for cumulus parameterization, 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 degree resolution were utilized. A one way nesting approach was chosen. Four dimensional data assimilation was utilized including assimilation of surface winds from surface observations. Model simulations were performed for the 11 July 1999 00 UTC to 25th July 1999 11 UTC period. The output frequency of the MM5 model was set to one hour.

*Comparison of MM5 model with NEOPS observations*

In order to assess the performance of the MM5 model with 14 layers in the vertical direction the above model results were compared with NE-OPS observations. In 1999 both C-172 as well as Aztec aircrafts were utilized during day and night periods in 52 spirals and 21 flybys during the operational period between July 4 to August 17, 1999. In situ observations of GPS position, standard meteorological (temperature, relative humidity at different pressure and altitude levels) and important atmospheric chemical tracers such as $O_3$ and CO were made from the instrumented aircraft. Since MM5 output was available every hour (0, 1, 2 UTC etc.), it was decided to compare the model output with the aircraft observations when the latter was in one of its spiral paths, either descending or ascending, and coinciding with the model output time. All the aircraft meteorological observations (temperature, relative humidity) were available at altitudes above mean sea level. Also the latitude and longitude of the aircraft position was available at various altitudes above mean sea level in its ascending or descending spiral paths. Utilizing the postprocessor GRAPH module of the MM5 model, the temperature and dew point temperature profiles at the aircraft locations were obtained and relative humidity calculated from the temperature and dew point temperature values. Next the grid cell closest to the latitude and longitude of aircraft location was identified and the terrain heights as well as the half sigma level heights of the four nearest grid cells were averaged and added to provide for the heights of the model levels above mean sea level at the aircraft locations. The temperature and relative humidity values of that model level closest to the aircraft altitude were extracted and assigned the appropriate height above mean sea level of that model level. All heights referred in the figures refer to heights above mean sea level. A similar procedure was employed for comparison of MM5 model results with other measurements such as RASS, wind profiler, lidar and tethersonde balloon except that unlike the aircraft case here it was a case of a single latitude longitude position of the measurement platform.

The comparisons of MM5 model results with 1999 NEOPS observations are depicted in Figure 2 (RASS July 19, 00 UTC), Figures 3a and 3b (aircraft July 19, 16 UTC), Figures 3c and 3d (wind profiler July 19, 17 UTC), Figures 4a and 4b (lidar July 17, 04 UTC) and Figures 4c-4f (for tethersonde balloon July 15, 21 UTC). Due to considerations of brevity we present one figure for comparison with each meteorological observation platform (a more detailed report can be found at http://www.ccl.rutgers.edu/techreports.htm). Temperature values obtained from aircraft are successfully reproduced by the model while this is not the case with the relative humidity values obtained from aircraft. The model tends to underestimate the relative humidity values especially in the lower atmosphere. The virtual temperature profiles predicted by the model compare very well with RASS data (Figure 2) while the wind components calculated by the model are only in partial agreement with the wind profiler data (Figures 3c and 3d). However the mixing ratio profiles and temperature profiles obtained from lidar data compare well with the model results (Figures 4a and 4b). The model predicted meteorological variables are only in partial agreement with the tethersonde balloon observations with relative humidity and wind speed being underestimated by the model.

## 3. AIR QUALITY MODELING

US EPA's Community Multiscale Air Quality (CMAQ) model, a component of the Models-3 system, and MCNC's Multiscale Air Quality Simulation Platform (MAQSIP) (Odman and Ingram, 1996) were used to simulate gaseous and aerosol phase air quality dynamics for the same domain. The modal aerosol model included as part of the current release of CMAQ was used in the CMAQ simulations while the dynamic sectional aerosol developed at the University of Delaware (UDAERO) (Sun and Wexler, 1998a, 1998b) was adopted in the MAQSIP simulations. The emissions data were processed from the National Emissions Trends (NET) (US EPA, ftp://ftp.epa.gov/EmisInventory) inventory using MCNC's Sparse Matrix Operator Kernel Emissions (SMOKE) (Houyoux and Vukovich, 1999) modeling system. The horizontal and vertical structures adopted were the same as for the meteorological model, with the number of cells six less than the corresponding MM5 grid in each horizontal direction, as required by the CMAQ and MAQSIP models.

Figures 5 and 6 show selected results from the comparison of CMAQ with observation data. An extensive set of comparisons for CMAQ as well as for MAQSIP can be found in the full report available at the website mentioned above. Figure 5 shows the comparison of total $PM_{2.5}$ mass predictions from the CMAQ simulations versus monitor data collected from five AIRS (http://www.epa.gov/airs/) monitor stations located in New Jersey (Bergen, Camden, Essex, Middlesex and Union counties) and those collected at the NE-OPS site in North Philadelphia by the Harvard School of Public Health. The model appears to capture the basic trends during the course of two weeks, however, with considerable under-predictions during the July 17-20 and July 24-25 episodes. Figure 6 shows the corresponding comparison for $O_3$. We can see that despite under-prediction of certain peaks the general agreement is quite good.

## 4. CONCLUSIONS

A comparative study of the evaluation of MM5 model with aircraft, lidar, tethersonde balloon, wind profiler and RASS observations obtained through NE-OPS over Philadelphia during one of the major summer episodes in 1999 was performed. The results of this study seem to indicate that the MM5 model performs well in capturing the mesoscale structure of the atmosphere for the period considered. Comparison with aircraft observations reveal that the temperature values are generally well simulated by the model while the same cannot be said of the relative humidity values. While the virtual temperature profiles predicted by the model compare very favorably with the RASS sounder data, the agreement of the horizontal wind components predicted by the model with the wind profiler data is only partial. The mixing ratio and temperature profiles obtained from lidar compare well with the model results. The MM5 model predicted meteorological variables are also only in partial agreement with the tethersonde balloon observations with both relative humidity and wind speed being underestimated by the model. The CMAQ model was found to be able to predict pollutant concentrations with a considerable degree of success. As expected, the prediction of $O_3$ was generally better than the prediction of $PM_{2.5}$. This is probably due to the fact that the physical and chemical processes associated with the formation of ambient $O_3$ are much better known than those associated with the formation and accumulation of $PM_{2.5}$. Also, the uncertainty in the primary PM emission inventory is probably larger than that for ozone precursors. On-going studies aim to identify relative contributions to PM mass of different processes by examining size-resolved and speciated PM predictions.

**Acknowledgement** The authors acknowledge the efforts of all group members of the NARSTO-NE-OPS research campaign in collecting and maintaining data from the various advanced research platforms. The authors also acknowledge NCAR for making the MM5 model available in the public domain and ECMWRF for providing the global analysis data.

## REFERENCES

Byun, D. W. and J. K. S. Ching: 1999, Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. U.S E.P.A. report EPA/600/R-99/030.

Clark, R.D.:2000, Measurements of PM2.5, O3 , and meteorological variables obtained using tethered balloons during the NARSTO-NE-OPS 1998 pilot study. Proceedings of the PM2000: Particulate Matter and Health Conference, Air & Waste Management Association, 6-7.

Doddridge, B.G.:2000, An Airborne study of Chemistry and fine particles over the U.S. Mid-Atlantic region. Proceedings of the PM2000: Particulate Matter and Health Conference, Air & Waste Management Association, 4-5.

Grell, G.A., J. Dudhia, and D.R. Stauffer: 1994, A description of the Fifth-Generation Penn State NCAR Mesoscale Model (MM5), NCAR Technical Note, NCAR TN-398, National Center for Atmospheric Research, Boulder, Colorado, 138 pp.

Houyoux, M., R. and J. M. Vukovich: 1999, Updates to the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System and Integration with Models-3. Presented at The Emission Inventory: Regional Strategies for the Future, 26-28 October, Raleigh, NC, Air & Waste Management Association.

Mulik, K.R., C. Li, G.S. Chadha, C.R. Philbrick, and S. Mathur: 2000, Evolution of Air Pollution events determined from Raman lidar. Proceedings of the PM2000: Particulate Matter and Health Conference, Air & Waste Management Association, 11-13.

Odman, M. T., and C. L. Ingram: 1996, Multiscale Air Quality SImulation Platform (MAQSIP): Source Code Documentation and Validation, ENV-96TR002-v1.0. Available from MCNC, 3021, Cornwallis Rd., Research Triangle Park, NC 27709.

Philbrick, C.R., R.D. Clark, P. Koutrakis, J.W. Munger, B.G. Doddridge, W.C. Miller, S.T. Rao, P. Georgopoulos, and L. Newman: 2000, Investigations of Ozone and Particulate Matter Air Pollution in the Northeast. Proceedings of the PM2000: Particulate Matter and Health Conference, Air & Waste Management Association, 1-3.

Sun Q. and A. S. Wexler: 1998a, Modeling Urban and Regional Aerosols—Condensation and Evaporation near Acid Neutrality. Atmospheric Environment 32, 3527-3531.

Sun Q. and A. S. Wexler: 1998b, Modeling Urban and Regional Aerosols near Acid Neutrality —Application to the June 24-25 SCAQS Episode. Atmospheric Environment 32, 3533-3545.

United States Environmental Protection Agency, National Emissions Trends (NET): ftp://ftp.epa.gov/EmisInventory


Figure 1. The triply nested MM5 modeling domain with the 36km (D01), 12km (D02) and 4km (D03) horizontal grid structure.

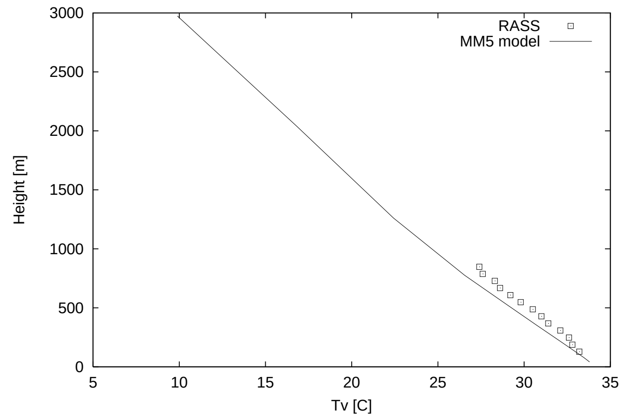



Figure 2. Comparison of NEOPS RASS virtual temperature observations with MM5 model results over Philadelphia for July 19 1999; 00 UTC.

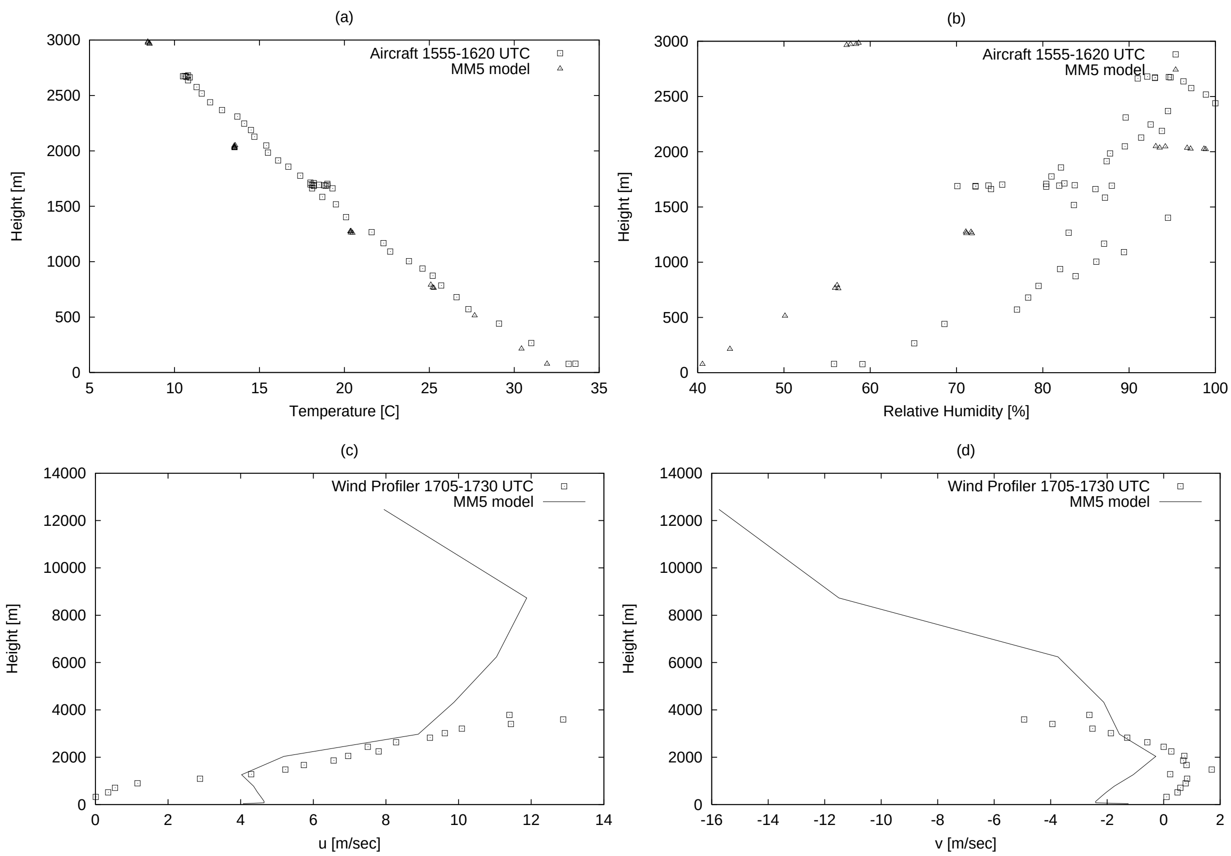



Figure 3. Comparison of MM5 model results with NEOPS aircraft observations on July 19 1999, 16 UTC (a, b) and NEOPS wind profiler observations on July 19, 1999, 17 UTC (c, d) over Philadelphia.

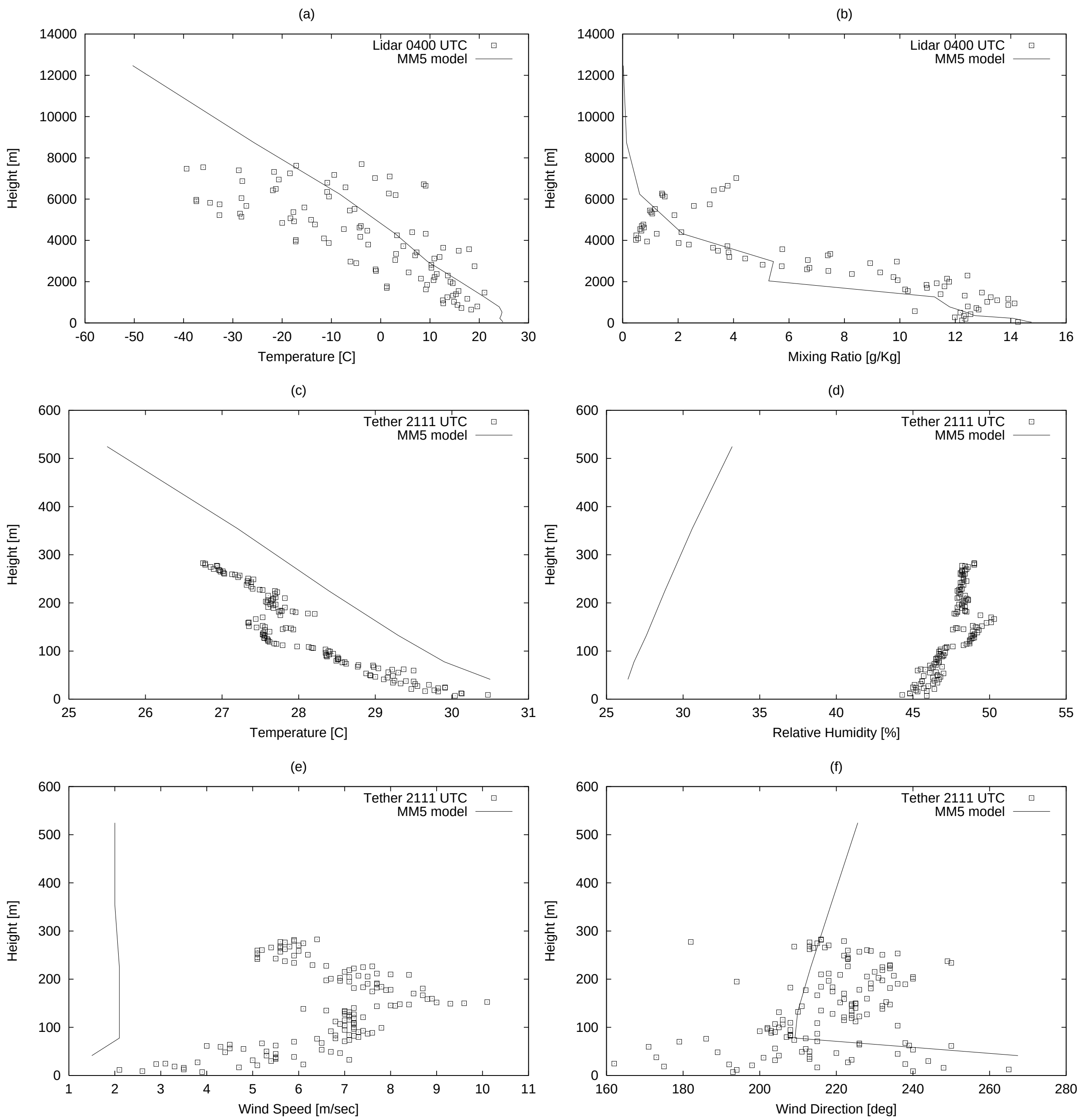
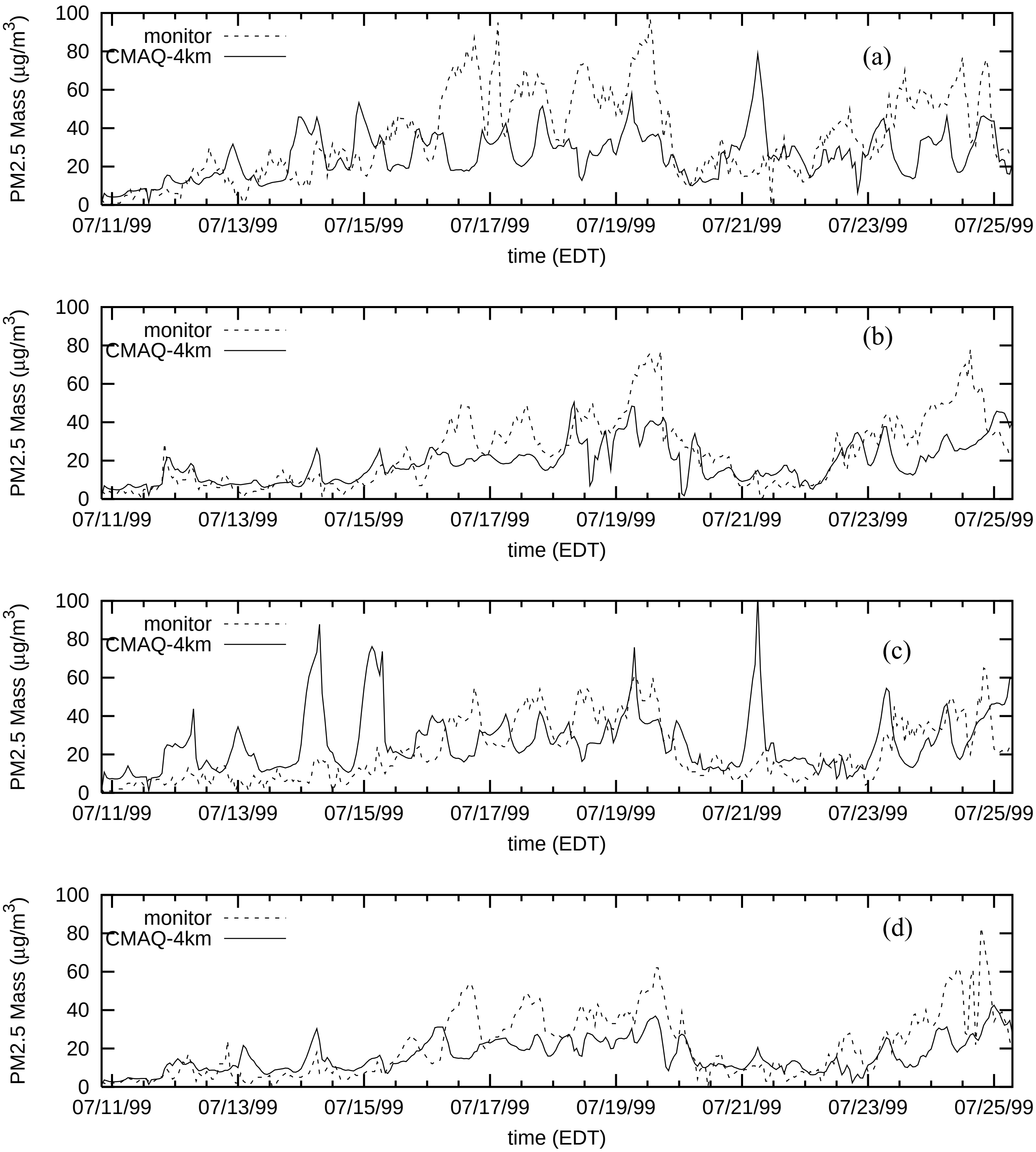



Figure 4. Comparison of MM5 model results with NEOPS lidar observations on July 17 1999, 04 UTC (a, b) and NEOPS tethered balloon observations on July 15, 1999, 21 UTC (c, d, e and f) over Philadelphia.


PM2.5 Mass (μg/m3)
monitor
CMAQ-4km
(a)
(b)
(c)
(d)
0
20
40
60
80
100
07/11/99
07/13/99
07/15/99
07/17/99
07/19/99
07/21/99
07/23/99
07/25/99
time (EDT)

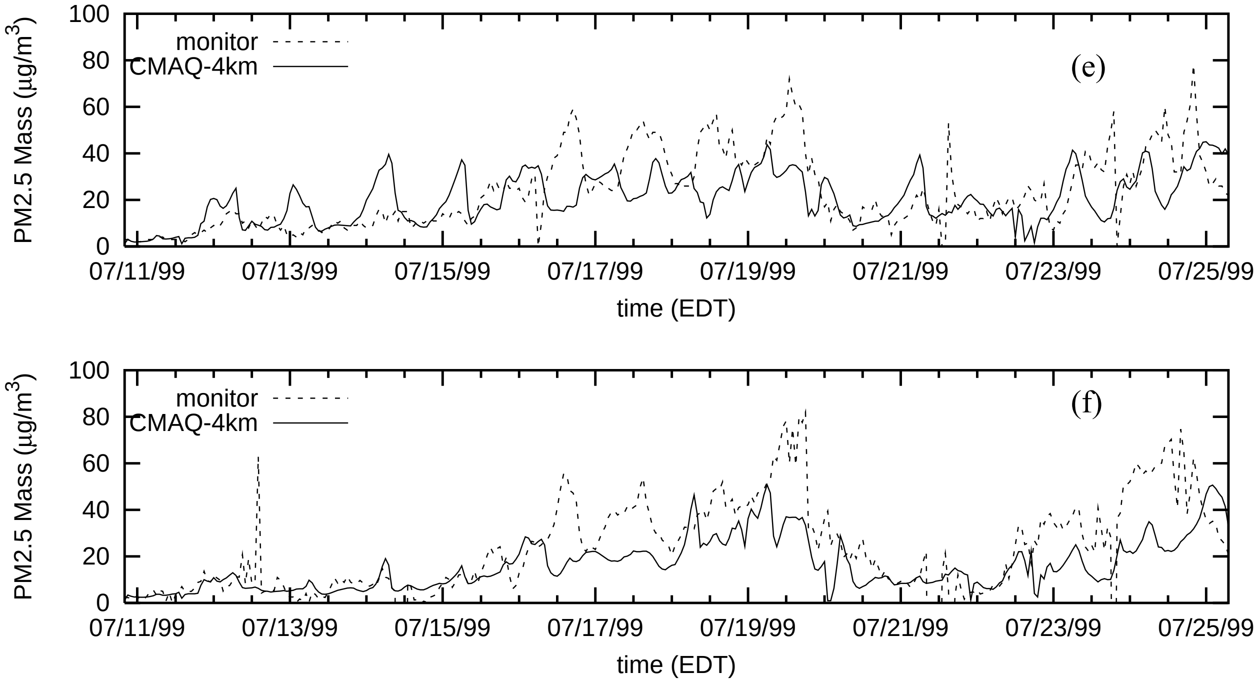



Figure 5. Comparisons of 4km resolution CMAQ PM2.5 predictions with observation data for (a) Bergen, NJ, (b) Camden, NJ, (c) Essex, NJ, (d) Middlesex, NJ, (e) Union, NJ and (f) Philadelphia, PA. The monitor data for Philadelphia is taken from the measurements of Harvard SPH during the NEOPS study and that for the rest are all taken from EPA's AIRS database.

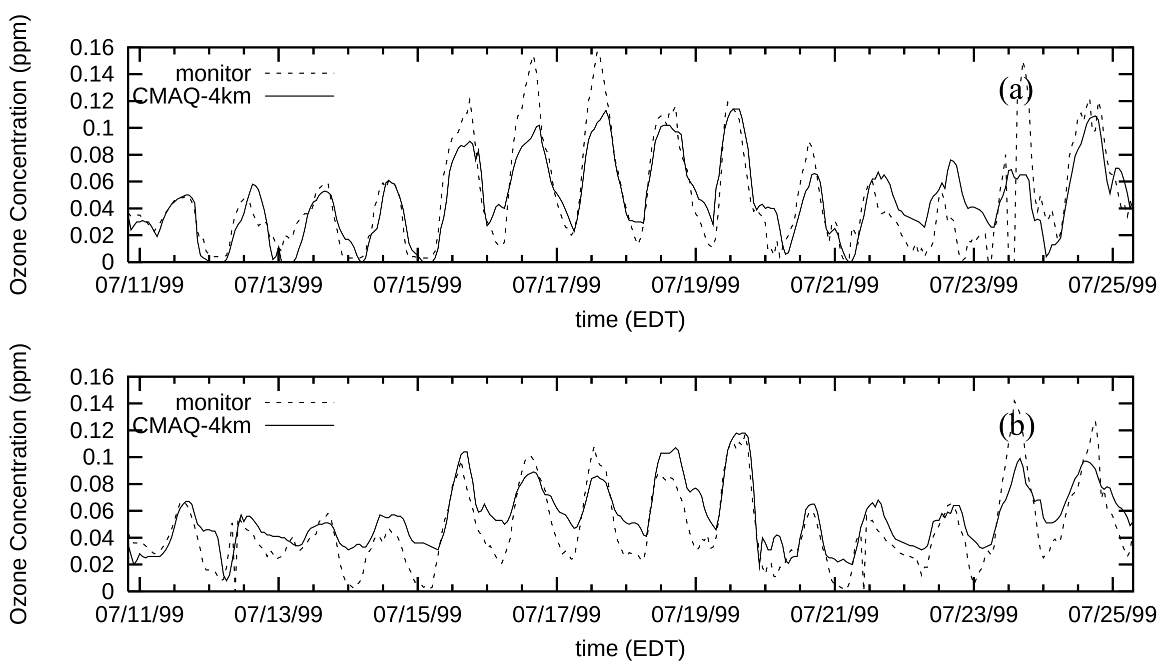



Figure 6. Comparisons of 4km resolution CMAQ ozone predictions with observation data for (a) Middlesex, NJ and (b) Camden, NJ. The monitor data is taken from EPA's AIRS database.