EVALUATING OZONE PREDICTIONS FROM PHOTOCHEMICAL MODELS USING NE-OPS 1999 OBSERVATIONS

Qing Sun, Anatharaman Chandrasekar, Panos G. Georgopoulos*
Environmental and Occupational Health Sciences Institute (EOHSI), a joint project of UMDNJ - R. W. Johnson Medical School and Rutgers the State University

C. Russell Philbrick
Penn State University, Department of Electrical Engineering and Applied Research Laboratory, University Park, PA, USA

Bruce Doddridge
University of Maryland, Department of Meteorology, College Park, MD, USA

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 by USEPA to improve current understanding of the underlying causes for the occurrence (and concurrence) of high ozone and fine particle concentration levels 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 summers of 1998 and 1999 (Philbrick, 2000).

Fast et al. (2002) evaluated an Eulerian chemical transport model developed at PNNL against NE-OPS data obtained during the period July 23 to August 11, 1999. The present investigation was primarily focused on a major ozone episode that took place in July 15-19, 1999 over the Philadelphia region, to perform an extensive evaluation of two widely used regional/multiscale photochemical models, namely, CMAQ (Byun, 1999) and CAMx (ENVIRON, 2002), in predicting ozone concentration by comparing model outcomes with both surface measurement data from USEPA's Aerometric Information Retrieval System (AIRS) and upper air aircraft data available from the NE-OPS study (Doddridge, 2000).

* *Corresponding author address:* Panos G. Georgopoulos, Environmental and Occupational Health Sciences Institute (EOHSI), 170 Frelinghuysen Road - Busch Campus, Piscataway, NJ 08854, Email: panosg@fidelio.rutgers.edu, Phone (732) 445-0159, fax (732) 445-0915

2. PROBLEM SPECIFICATIONS

The simulations for this study were carried out for the July 11, 1999 00 UTC to July 25, 1999 12 UTC period. Three levels of nested grids were used with grid resolutions of 36km, 12km and 4km (see Figure 1). The 36km grid encompasses the Eastern United States while the 4km grid encampasses the Philadelphia - New Jersey region. In the vertical direction, the CMAQ application used a non-hydrostatic coordinate with 14 layers centered at 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 in sigma-p units, while the CAMx application used 8 layers corresponding to the lowest 8 layers for the CMAQ simulations.

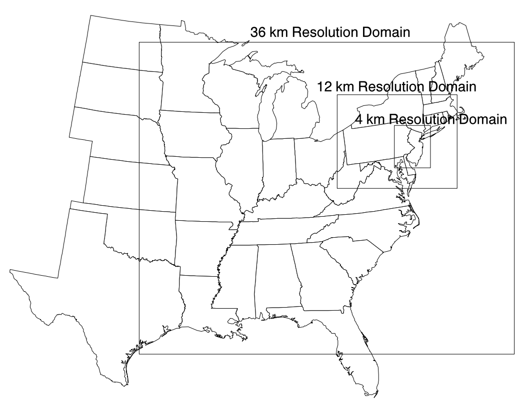

Figure 1. Nested air quality modeling domains with 36km, 12km and 4km horizontal grid resolutions employed in the present study.

In order to obtain the meteorological inputs, simulations were performed with the Fifth Generation Pennsylvania State

University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) (Grell, 1994) model for the nested multiscale model domain and for the duration of the modeling period. Details of the MM5 simulations can be found in Chandrasekar et al. (2002a,b, 2003).

The emissions data were processed from the National Emissions Trends (NET) (USEPA, 1999) inventory using MCNC's Sparse Matrix Operator Kernel Emissions (SMOKE) (Houyoux, 1999) modeling system.

The ozone concentration data from AIRS and from the monitor station at Philadelphia Air Management Services Laboratory, made available through the NE-OPS study, were used for comparisons with the model predicted ozone values. The upper air ozone data used for comparison with model prediction were taken from the University of Maryland instrumented flights with Cessna and Aztec aircrafts (Doddridge, 2000).

3. RESULTS

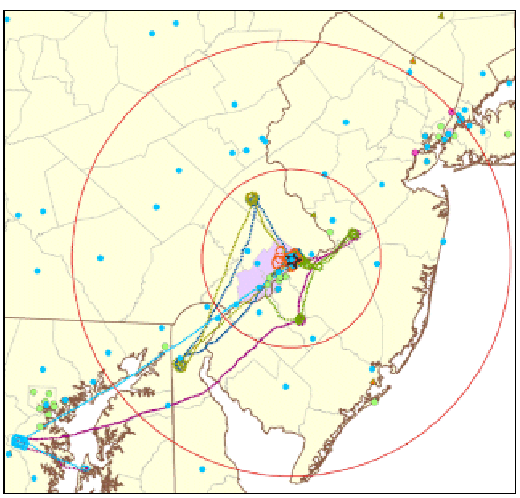

Figure 2. Air quality monitoring stations and flight tracks in the vicinity of NE-OPS. The circles indicated in the figure correspond to a radius of 50 Km and 100 Km with the Baxter NE-OPS site at the center.

Figure 2 shows the air quality monitoring stations and flight tracks in the vicinity of NE-OPS Baxter site. Also depicted in the same figure (in purple) is the area representing urban Philadelphia, the region representing the focus of a population exposure study to Ozone and fine Particulate Matter during the summer period of 1999 (Georgopoulos et al., 2003).

Both CMAQ and CAMx simulations were performed for the three levels of nested grids. Figure 3 shows the daily maxima of ground level ozone spatial distributions for 7/17/1999, as predicted by CMAQ and CAMx, respectively, over the 4km resolution domain; one can see that CAMx predicts higher peaks while CMAQ predicts wider extent of ozone. Figure 4 presents space-time paired plots and quantile-quantile plots for ground level ozone concentrations observed at fourteen AIRS ozone monitor stations in New Jersey and one NE-OPS station at Philadelphia during July 11-25, 1999, versus model predictions by CMAQ and CAMx, respectively, at the locations of those monitor stations, at the hours when those monitor data were collected. One can see that for the middle range of concentrations the two models calculate similar concentration values but for the lower concentration range the CMAQ predictions tend to be higher than those of CAMx while for the high concentration range CAMx tends to overpredict ozone values.

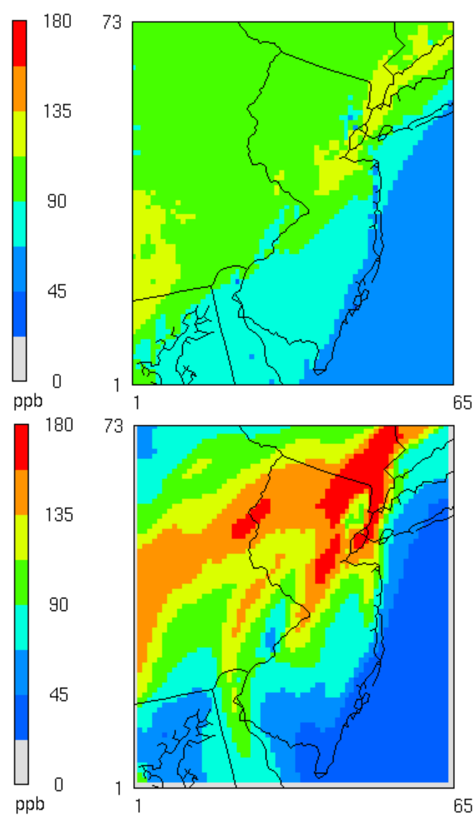

Figure 3. Daily maxima of ground level ozone spatial distributions for 7/17/1999 predicted by CMAQ (upper) and CAMx (lower) for the 4km resolution grid.

Figure 5 shows comparisons of 4km resolution CMAQ and CAMx ozone time series predictions with observed data from monitors located in Middlesex, NJ and Philadelphia, PA. The observation data for Philadelphia were obtained from the NE-OPS study, while those for NJ are from USEPA's AIRS database. One can see an over-prediction of ozone by CAMx on certain high ozone days for Middlesex.

Figure 6 shows comparisons of upper air predictions of ozone concentrations from both CMAQ and CAMx with aircraft data collected during the NE-OPS study on a flight on July 18, 1999. One can see for the July 18 evening flight, that both model predictions agree with the measurement data for altitudes in the range of 200-600 m, and both under-predict, to a different degree, for altitudes higher than 700m and also at the surface.

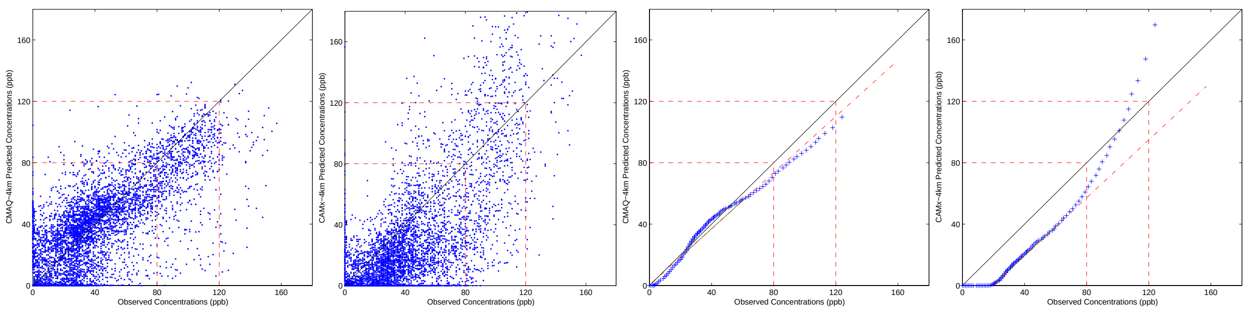

Figure 4. Space-time paired comparisons and quantile-quantile plots of ground level ozone concentrations during July 11-25, 1999 over the 4 km resolution domain: the observation data were measured at 14 AIRS stations located in New Jersey plus the NE-OPS station located in Philadelphia: (a) observed versus CMAQ predicted, space-time pairs; (b) observed versus CAMx predicted, space-time pairs; (c) observed versus CMAQ predicted, quantile-quantile; (d) observed versus CAMx predicted, quantile-quantile.

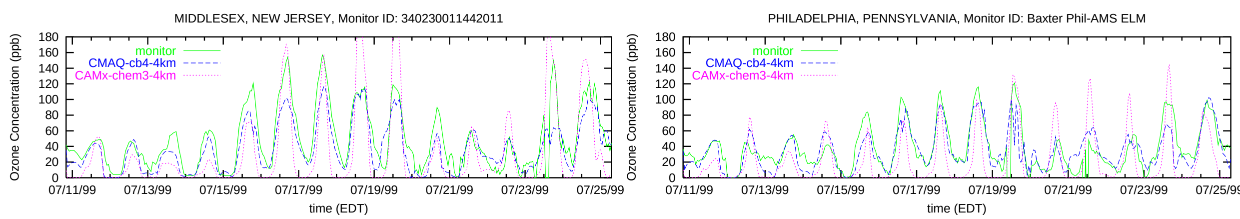

Figure 5. Ozone time series comparisons between CMAQ and CAMx 4km resolution model predictions and observation data for Middlesex, NJ and Philadelphia, PA. The observation data for Philadelphia were obtained from the NE-OPS study, while those for Middlesex, NJ are from USEPA's AIRS database.

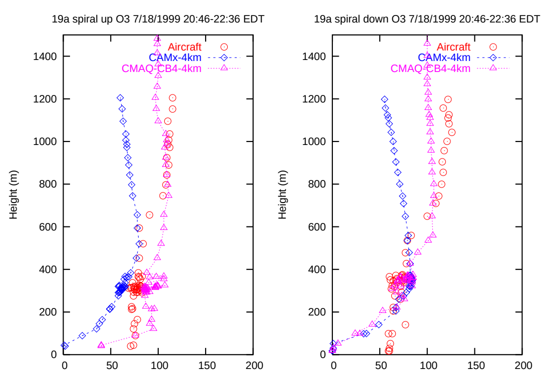

Figure 6. Comparison of 4 km resolution CMAQ and CAMx ozone predictions with flight measurements on 7/18/1999 20:46-22:36 EDT. (left panel: spiral up; right panel: spiral down)

4. CONCLUSIONS

The comparisons of CMAQ and CAMx model predictions with surface measurement data from AIRS and NE-OPS show relatively reasonable agreements for ozone predictions. The model predictions capture the general trends of change in the time series plots. Considerable discrepancies can be seen from the comparison of upper air model predictions and aircraft measurement data. It is therefore necessary to further examine the options and assumptions underlying the application of these models in order to identify the causes of this discrepancy; though it may be reasonable to assume that the use of a higher number of layers in the CMAQ application (fourteen layers) versus that in the CAMx application (eight layers), which was made to reflect typical practice in the application of the two models, explains the better agreement of CMAQ results with upper air observation, further investigation of this issue is necessary.

ACKNOWLEDGMENTS

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