MODELS-3/CMAQ EVALUATION DURING HIGH PARTICULATE EPISODES OVER EASTERN NORTH AMERICA IN SUMMER 1995 AND WINTER 1998

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INTRODUCTION

The performance of the US Environmental Protection Agency (EPA) air quality modelling system MODELS-3/CMAQ/MM5 has been evaluated during high particulate episodes which occurred over eastern North America on July 9 – 17, 1995, and February 5 – 13, 1998. The Community Multiscale Air Quality (CMAQ) is a third generation chemical transport model for urban to regional scale simulation of ozone, acid deposition, and fine particulate matter. The meteorological driver for CMAQ is MM5 – the Pennsylvania State University/NCAR meso-meteorological model.

Emissions from US and Canadian inventories were processed for a modeling domain with 36 km resolution with 30 vertical levels that go up to 100 hPa. The domain covers the eastern part of North America – from Florida in the south to Hudson Bay in the north, and from North Dakota in the west to Newfoundland in the east.

Modelling results for $PM_{2.5}$, PM_{10}, secondary aerosols and precursor gases (SO_2, NO_2) were compared with observed data derived from a number of networks of monitoring stations operated in the USA and Canada during the episodes. Model evaluation techniques applied included scatter plots, calculation of temporal and spatial correlation coefficients, bias, index of agreement, RMSE, gross error and visual analysis. The results of these evaluations are presented in this study.

EPISODES DESCRIPTIONS

February 1998 episode extended over southern Ontario, Quebec and the northeastern US and was dominated by a high-pressure system under stagnant atmospheric conditions. During the episode surface temperatures were above 0^oC and no precipitation was observed. Circulation at 850 mb brought warm air northward increasing static stability in the lower troposphere, reducing mixing in the boundary layer. The episode ended with the passage of a cold front on February 13.

Observed data from the US and Canadian networks showed the maximum PM_{10} levels were recorded on February 10. On this day the 24-hour averaged concentrations reached 107 ug/m^3 in the Syracuse and 135 ug/m^3 in Cleveland areas. On February 11, 138 ug/m^3 was observed in Montreal area. In general, the multi-day build-up of the stagnation episode began on February 7 and proceeded through February 11.

From July 7 to July 10, the eastern part of the continent was dominated by an elongated trough, which slowly moved northeastward towards the Atlantic with surface pressure rising in its wake. On July 12, a Bermuda High extended over eastern Canada and the US leading to conditions that are favourable for development of summer particulate episodes: weak winds, high temperatures, vertical descent, clear skies and low inversions. This high-pressure system persisted for the next

2-3 days until a cold front from Northern Ontario swept through the area bringing precipitation and clean and cool northerly air.

On July 14, daily PM_{10} concentrations higher than 50 ug/m^3 were widely observed over the eastern US covering an area from Tennessee and Kentucky to the East Coast.

MODELLING DESIGN

In this study we used MM5 as the meteorological driver, MEPPS (Models-3 Emission Processing and Projection System) for emission processing and CMAQ as the chemical transport model.

In MM5 parameterization of the boundary layer has been done using the Blackadar scheme, with the Kain-Fritsch scheme coupled with a mixed phase explicit scheme used for moist processes (*MM5 Modeling System Version 3, NCAR*, 2002). 36-hour forecasts were calculated for every day of the episodes with a spin-up period of 12.

The Canadian emission inventory has been considerably improved compared to that originally supplied with Models-3 database. The improvements included:

- New, annual average emission inventories for point, area and mobile sources for 1995 were put into MEPPS
- Canadian area and point source temporal allocation factors were added to the temporal lookup table.
- Information on the distribution of crop and forest species in Canada was integrated with land use data to provide better input to the BEIS-2 model.
- For eastern Canada, MOBILE5a input files were replaced with province specific1995 data.
- Population and dwelling data by census enumeration area was put into MEPPS to replace the much coarser census division data originally in the database.

CMAQ's set-up used mostly the default modules along with the RADM-2 chemical mechanism including aerosol and aqueous chemistry (*D.W.Byun and J.K.S. Ching*, 1999). Observed data was used to set up time dependent inflow boundary conditions.

RESULTS AND DISCUSSION

The results of CMAQ runs were evaluated against extensive observed data, derived from several US and Canadian networks. Evaluation of the model was performed in the domain reduced by 3 cells (108 km) from each boundary. The model was run with a 2-day "warm up" period, during which the results were not analyzed.

July 1995 evaluation

Figure 1 presents scatter plots for modelled versus observed 24 hour average PM_{10}, $PM_{2.5}$, SO_4, NO_3 and NH_4. Modelled sulphate concentrations were strongly correlated to observed data and showed very little bias. PM_{10}, $PM_{2.5}$ and ammonium were also strongly correlated with observed data however the model results are slightly lower than observed data on average. Modelled nitrate was higher then observed data however a number of the nitrate measurements could be biased low because of volatilization losses. Similar analyses of some of the precursor gases shows nitric acid predictions to be strongly correlated to measured data but biased high relative to the data. Measured and modelled concentrations of SO_2 and NO_2 were correlated with modelled SO_2 results tending to be biased slightly high and NO_2 biased slightly low.

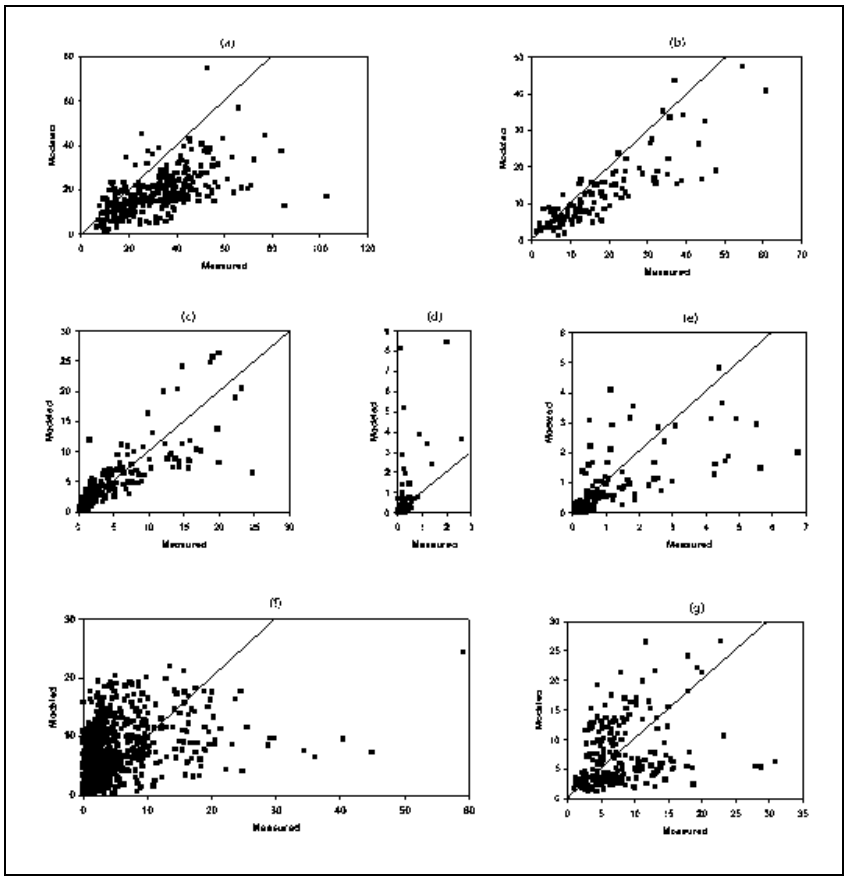

Figure 1. Scatter plots of modelled vs. observed surface concentrations (ug/m^3) for July 9-17, 1995: a) PM_{10}, b) $PM_{2.5}$, c) SO_4, d) NO_3, e) NH_4, f) SO_2, g) NO_2.

Time correlations were calculated at sites with at least 5 days of observations. Modelled time series for sulphate and ammonium were strongly correlated with observed data at a large majority of the sites (0.75 to nearly 1). Both species demonstrate the same spatial pattern with maximum correlations in Quebec and a gradual decrease in the west direction.

The comparison of CASTNET data (weekly observations) versus averaged modelled data for SO_4, NH_4 and SO_2 shows almost an exact match in the locations of maximums for all species, with SO_4 and NH_4 matching measured values. Modelled SO_2 concentrations are biased very high (order of magnitude), but the spatial correlation is excellent.

February 1998 evaluation

Ammonia emission rates have no seasonal variability in MEPPS. That results in a significant overestimation in February since manure spreading, the largest source of ammonia emissions, is not occurring in northeastern North America at that time. This is very important for the winter episode, which is dominated by formation of ammonium nitrate. A model run with emissions of NH_3 reduced by 50 % shows improved comparisons with observed data. Figure 2 shows scatter

plots for NO_3 and NH_4 for the base case NH_3 emissions and half NH_3 emissions. In both cases NO_3 is biased high, but the magnitude is much better with half ammonia emissions and NH_4 shows very good correspondence with observations.

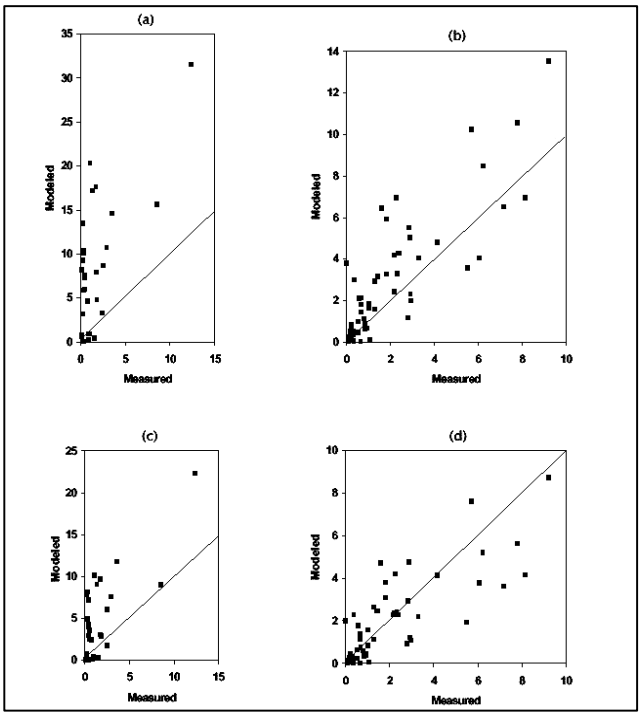

Figure 2. Scatter plots of modelled vs. observed surface concentrations (ug/m^3) for February 5-13, 1998: a) NO_3 and b) NH_4 with base case emissions and c) NO_3 and d) NH_4 with half NH_3 emission rates.

Figure 3 presents scatter plots of modelled vs. observed surface concentrations for particulate matter, sulphate, SO_2 and NO_2. PM_{10} is biased slightly low, and PM_{25} is biased high against the observations. Modelled sulphate concentrations are correlated with observed data but are biased low relative to the measurements. Scatter plots for SO_2 and NO_2 give good correlations between modelled and observed concentrations. The modelled SO_2 is biased high by about 50%. Modelled NO_2 concentrations are highly correlated with measured data and show very little bias.

The time series correlation coefficients for sulphate and ammonium are lower than was found for the summer episode but are still between 0.5 and 0.95 at a large majority of the sites. Sites in southern Ontario had time correlation coefficients in 0.8 to 0.95 range with sites in Quebec having values between 0.3 and 0.75. The area of maximum correlation for ammonia is located just to the north of lake Huron. The magnitude of correlation smoothly decreases in the east direction. Maximum correlations for sulphate are in southern Ontario with the lower correlations in southern Quebec.

Very good correspondence can be seen between CASTNET weekly observations and modelled data both in the pattern of the contours and the magnitude for NO_3, NH_4 and SO_2. Areas with

maximum concentrations have basically the same locations. This shows up clearly for SO_2 concentration field, with modelled concentrations biased high, as was found for the summer episode. Modelled maximum concentrations for NO_3 and NH_4 are shifted to the east against observed data.

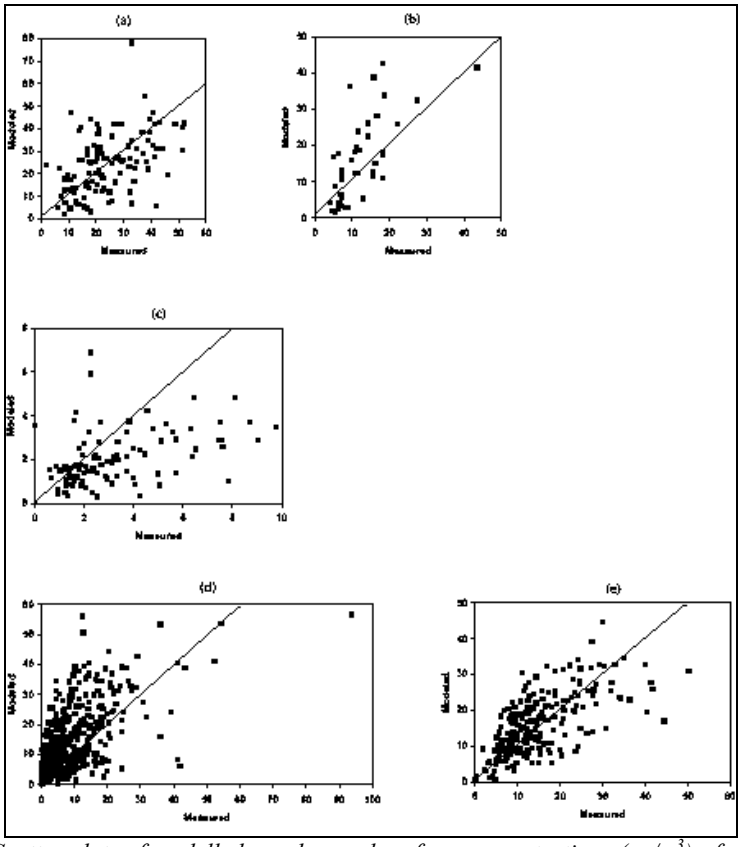

Figure 3. Scatter plots of modelled vs. observed surface concentrations (ug/m^3) for February 5-13, 1998: a) PM_{10}, b) $PM_{2.5}$, c) SO_4, d) SO_2, e) NO_2.

CONCLUTIONS

In general, the model demonstrates overall reasonably accurate predictions for particulate matter during both episodes, but some secondary aerosols and precursor gases tend to be biased either high and low versus measured data (up to 50% for SO2). Time correlation coefficients for a number of species were very high (up to 0.75 - 0.95). The model also captures spatial distributions of the surface concentrations, the timing of the evolution of the episodes, and the chemical composition of the aerosols.

REFERENCES

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

PSU/NCAR Mesoscale Modeling System Tutorial Class Notes and Users' Guide: *MM5 Modeling System Version 3, NCAR*, 2002.