1. INTRODUCTION

A regional air quality modeling study was performed for a typical summer smog episode that occurred in the Northeast of the United States and Southern Ontario from July 13 to 17, 1999. The general synoptic and weather conditions in Southern Ontario are favorable to smog/ozone formation according to previous studies (Mukammal, et al., 1981, Yap, et al., 1988). During the episode, the back side (western side) of a slow-moving high-pressure system was centered over the eastern coast of the U.S. In the area of the Ohio Valley, Southern Ontario and the Northeast coast, southwest surface winds dominated for days with moderate wind speeds. The surface temperature day-time high climbed from 25 to 35°C over the 5-day period. Weather conditions were mostly sunny, with a few clouds; scattered showers in the afternoon of July 15, and no thunderstorm in the study area until July 17. Smog Warnings were issued by Environment Canada during the episode.

MM5 was used to re-generate the meteorological fields with 36 km, 12 km and 4 km grid spacings. SMOKE was used to prepare the gridded emissions for air quality modeling. CMAQ was used to model photochemistry and transport of pollutants for all of three grids resolutions. There was a problem found in the preliminary results of the CMAQ modeling: predicted ozone levels in the 12 and the 4 km grid domains were underestimated significantly in the daytime, and overestimated in the nighttime. However, the primary and the non-photolysis pollutant levels were predicted relatively well (e.g. SO2, CO, etc.). To investigate the problem, a series of sensitivity tests were performed through MM5/SMOKE/CMAQ runs to check the emission input/output from SMOKE, the settings for CMAQ, the MCIP processor and the options used with MM5. For the MM5 sensitivity tests, the initial/boundary conditions, boundary layer schemes, land-surface schemes, FDDA processes, radiation schemes, cumulus parameterization and gridded cloud and precipitation schemes were examined individually.

2. SENSITIVITY TESTS

The sensitivity tests indicated that the over-predicted cloud cover fraction (as well as the cloud depth and the cloud top/base heights) from the MCIP output played an important role in the ozone under-prediction problem. Since CMAQ cannot use MM5 outputs directly, MCIP is used to convert the output from MM5 and prepare the various input meteorological files in formats consistent with the requirements of SMOKE and CMAQ. In the MCIP configuration, the cloud parameter module is the same module used in MM5-PX. A comparison between the MM5 cloud output and the MCIP cloud output was performed and the difference between the two outputs was minor. Therefore in this case study, the over-predicted cloud cover is actually due to the over-prediction of cloud cover in the MM5 runs.

Since ozone is formed through photochemical processes, the photolysis rates are the key factors to predict ozone concentrations. The photolysis rates in CMAQ require cloud correction factors (e.g. cloud coverage fraction and cloud transmissivity) from MCIP which is tightly linked to the MM5 output. The application of cloud correction factors to photolysis rates in CMAQ can be shown in the following equations (Byun and Ching, 1999):

\[
J_{\text{below}} = J_{\text{clear}} \left[ 1 + \text{cfrac}(1.6t_c \cos(\theta) - 1) \right]
\]

\[
J_{\text{above}} = J_{\text{clear}} \left[ 1 + \text{cfrac}(\alpha_c(1 - t_r) \cos(\theta)) \right]
\]

where,

- \( J_{\text{clear}} \) - clear sky photolysis rate for a specific date,
- \( J_{\text{below/above}} \) - photolysis rate below/above cloud,
- \( \text{cfrac} \) - cloud coverage fraction,
- \( t_r \) - cloud transmissivity, function of liquid water content (L) and cloud thickness (Dz).

If the cloud coverage fraction \( \text{cfrac} \) and the cloud transmissivity \( t_r \) are predicted incorrectly, the photolysis rates below/above clouds \( J_{\text{below/above}} \) will be calculated incorrectly, leading to the under/over-prediction of ozone levels.

The cloud prediction is related to the convective parameterizations and microphysics schemes used in MM5. In nature, convection not only produces precipitation, but also transports heat upward and downward and redistributes moisture, thereby stabilizing the atmosphere. The convective parameterization scheme used in the mesoscale model must try to account for these types of convective effects. In MM5, there are numerous convective and microphysics schemes available. The correct options selected in a simulation must correspond to the MM5 model resolutions, the weather conditions being modeled and the other correlated physics options.
3. RESULTS

In the preliminary MM5 runs (“Old”), the convective and the microphysics schemes were the Grell scheme (1994) + the mixed-phase scheme for the 36, 12 and 4 km grid spacing runs. However, over-predicted convection and clouds/precipitation in the 12 and 4 km runs indicate that the convective parameterization and microphysics options used were not suitable to this case study. In the “New” MM5 runs, the Kain-Fritsch scheme (1993) + the mixed-phase was applied to the 12 km grid run, and the convective parameterization option was turned off in the 4 km grid run. These changes to the cloud/precipitation schemes induced much better results regarding the cloud prediction in MM5.

Figure 1 shows an example of the comparison between the Old (left) and the New (right) MM5 runs in terms of the cloud coverage prediction at the 12 km grid spacing. On July 16, 1999 at 2000 GMT, the Old MM5 run predicted a large area of cloud over much of eastern U.S., Lake Erie and Lake Ontario, and part of Southern Ontario. Compared to the observations (RWDI, 2001), the cloud coverage in MM5 was over-predicted. However, the New run predicted a smaller area of clouds over the eastern U.S., a few clouds over Lake Erie, and none over Southern Ontario. This prediction is much closer to the observations.

Figure 2 shows a comparison between the CMAQ runs for ozone using Old and New MM5 outputs. The New CMAQ run predicted a 30% increase in ozone levels compared to the Old run. The predicted ozone levels and the spatial distribution patterns from the new CMAQ runs are much closer to the ozone monitoring data (RWDI, 2001). The 4 km grid simulations, although not shown here, depict similar conclusions as 12 km grid run.

4. CONCLUSIONS

Cloud cover/thickness prediction in MM5 is often overlooked in air quality studies, although it plays an important role in ozone prediction. The combination of the selected convective parameterization and the microphysics schemes can change the MM5 cloud/precipitation prediction considerably. In the 12 km grid run, the Kain-Fritsch convective scheme performs well in the July 1999 study. For the 4 km grid, the convective scheme should be turned off and the microphysics scheme should be used to resolve the cloud/rain water content. In higher resolution MM5 runs (e.g. 4 km grid or finer), the selection of the microphysics scheme may be sensitive from case to case in summer in terms of convection types. However, correct meteorological modeling relies on not only the cloud simulation, but also the boundary/initial conditions, boundary layer, radiation, land use, horizontal/vertical resolutions, FDDA, etc. Future study will continue on cloud/fog prediction which may also affect the formation of particulate matter (especially in the aqueous phase). More sensitivity tests of MM5/CMAQ are recommended.

6. REFERENCES


RWDI, 2001: Models-3 study in southern Ontario: Final Report (submitted to Environment Canada)