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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

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Office of Air Quality Planning and Standards
Research Triangle Park, NC 27711

DEC 15 1994

REPLY TO THE ATTENTION OF:
(MD-10)

Lake Michigan Air Directors Consortium
2350 East Devon Avenue, Suite 242
Des Plaines, Illinois 60018

Dear Lake Michigan Air Directors:

The United States Environmental Protection Agency (USEPA) received your October 1, 1994 letter and enclosure of the model performance evaluation results of the Urban Airshed Model, Version V for the Lake Michigan Region. USEPA is pleased with the extent of the technical work which the Lake Michigan States performed to achieve the "Basecase C" model results and with the cooperation between USEPA staff and the participants of the Lake Michigan Ozone Study.

After reviewing the technical support documentation, we have determined that the model submitted to USEPA is performing in an acceptable manner and may be used for regulatory purposes. A detailed discussion of USEPA's review of the model validation technical support documentation is contained in USEPA's enclosed technical review, dated December 15, 1994.

It should be noted that if the current model is modified, it will be necessary for USEPA to evaluate those changes. I appreciate the efforts you have made in this area and look forward to working with you to address this ozone problem.

Sincerely,

John Seitz, Director
Office of Air Quality Planning and Standards

Enclosure

cc: Donald Theiler, Director, Bureau of Air Management, Wisconsin DNR
Bharat Mathur, Chief, Bureau of Air, Illinois EPA
Dennis Drake, Acting Director, Air Quality Division, Michigan DNR
Timothy Method, Director, Office of Air Management, Indiana DEM
David Kee, Director, Air and Radiation Division, Region 5
Stephen Gerritson, Director, Lake Michigan Air Directors

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

DATE: December 15, 1994

SUBJECT: Technical Support Document: Review of the Lake Michigan Ozone Study's Basecase C Model Performance

FROM: Sheila P. Breen, Region 5
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Ed Doty, Region 5
Mary Onischak, Region 5
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THRU: Gary Gulezian, Chief
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On October 1, 1994, the Lake Michigan Air Director's Consortium (LADCO) submitted their latest evaluation of Urban Airshed Model-version V (UAM-V) performance. This evaluation included the results for Episodes 1, 2, 3 and 4 for Basecase C. Basecase C has the following model input configuration.

MODEL BASECASE INPUTS

Grid Configuration and Plume Algorithms

The source and receptor grid for the model include a nested grid system with the following horizontal grid resolutions: 16 kilometers (Grid A); 8 kilometers (Grid B); and 4 kilometers (Grid C) (see Figure 1 in the October 1, 1994, submittal for the locations of these grids). Eight vertical layers were modeled for the entire domain.

Plumes from the 50 largest (highest emitting) Oxides of Nitrogen (NOx) stationary sources are modeled with the Plume-in-Grid (PiG) algorithm, which represents plumes as a series of discrete Gaussian puffs. Outer layers of each puff (a puff is initially composed of four concentric layers) are dumped to the grid when the vertical cross-sectional areas of the layers equal or exceed the vertical cross-sectional area of a grid cell. An entire puff is dumped to the grid when the volume of the puff exceeds 1/2 times the volume of a grid cell in Grids A and B or exceeds the volume of a grid cell in Grid C.

Emissions

The Grid B and C emissions for the point and anthropogenic area sources were developed using the States' 1990 base year emission inventories as adjusted through subsequent State updates and corrections (the final correction phase has been referred to as Round 3a). The Grid B and C emissions for on-highway mobile sources were derived through the use of the Motor Vehicle Emissions Model (MoVEM) in the Geocoded Emissions Modeling and Projections System (GEMAP) (MoVEM produces emissions estimates by multiplying MOBILE5a emission factors times the vehicle miles travelled estimates for modeled traffic links). Grid B and C biogenic emissions were derived by the Biogenic Model for Emissions Estimation (BIOME) contained within GEMAP (BIOME basically applies USEPA's BEIS biogenics emissions model using updated land use/land cover data derived from LANDSAT imagery and an updated corn emission factor).

Grid A point and anthropogenic area source emissions were derived from the USEPA 1990 Interim Regional Inventory for the States of Illinois, Indiana, and Michigan and statewide emissions provided by the State of Wisconsin. Grid A biogenic emissions were derived using USEPA's BEIS, hourly temperatures for a representative, hot summer day (July 5, 1988), the updated emission factor for corn, and land use data obtained from the Oak Ridge National Laboratory's GEOECOLOGY data base. Grid A on-highway mobile source emissions were derived using 1990 Highway Performance Monitoring System areawide vehicle miles travelled data and MOBILE5 emission factors.

All emissions data were processed by the GEMAP to derive temporally, spatially, and specially resolved data for input into UAM-V.

Meteorology

Wind fields were developed using the CALRAMS 2c model. Wind speed corrections (minimum wind speeds of 3 meters per second in the Grand Rapids, Michigan area) were made for certain days of Episode 4 outside of the CALRAMS 2c model results. Episode 2 required day-specific examination of cloud conditions.

The vertical mixing was done on a gridded basis (KRAMS), and a factor of 3 increase was required for correcting prior contractor assumptions which suppressed vertical mixing. The minimum vertical mixing was increased to be consistent with the other air quality and meteorological models. Diurnal patterns of vertical mixing were modified to smooth the transition during the early morning and late afternoon. An urban heat island/potential temperature gradient was considered for those grid cells with at least 30% urban land use/land cover. Plumes of elevated shoreline sources were maintained and "F" stability was assumed for all PiG plumes over the Lake or along the lakeshore.

Boundary and Initial Conditions

Based on the 1991 field study measurements, boundary conditions (VOC, carbonyls, and NO_x) for the first two modeled layers were obtained from the actual surface measurements from all episodes. The boundary conditions for the upper six layers were obtained from the actual aircraft measurements for Episodes 1 and 2. NO_y inputs, based on research information, were found to be two times as great as the observed NO_x values, (which were assumed to be mostly NO, NO_2, and some PAN. The NO_y breakdown was a 0/40/20/40 split for $NO/NO_2/PAN/HNO_3$.

Atmospheric Chemistry

Atmospheric chemistry was analyzed as a part of LMOS's on-going sensitivity analyses. One such analysis displayed that the UAM-V, using the photolysis rates from USEPA's guideline photochemical grid model, UAM Version IV,
(UAM-IV) gave the most realistic results compared to actual monitored concentrations, especially along the lakeshore area. Both versions of the model rely on the same chemistry, known as the Carbon Bond IV chemical mechanism (CB IV). UAM-IV rates with the CB IV mechanisms are a part of the recommended guideline model, but UAM-V is preferred for the LMOS domain because of its ability to treat lakeshore effects.

Episode Days

During the study days of Episode 1, June 26th through June 28th, winds were south-southwesterly, with a peak ozone concentration of 175 ppb in Manitowoc, Wisconsin. Episode 2's study days, July 17th through July 19th, had southwesterly winds, with peak ozone concentrations of 170 ppb occurring in Holland and Sleeping Bear Dunes National Lakeshore, Michigan. The Episode 3 study days of August 25th through August 26th had a peak 1-hour concentration of 189 ppb near Milwaukee, Wisconsin. Light winds started out in the beginning from the southeast on this episode, and ended up being from the south. June 20th and 21st represented the study days for Episode 4, with easterly to northeasterly winds and a peak ozone concentration of 152 ppb in Cary, Illinois.

PERFORMANCE CRITERIA GUIDANCE

USEPA requires UAM applications to meet specific model performance criteria before they are considered acceptable for regulatory purposes. The Guideline for Regulatory Application of the Urban Airshed Model (Guideline) outlines a series of performance tests which are designed to help assess overall model performance in replicating observed ozone concentrations and patterns. These tests include both quantitative (i.e., statistical) and qualitative (i.e., graphical) analyses.

At a minimum, the Guideline recommends the following statistical tests:

Unpaired peak prediction accuracy - This test quantifies the difference between the highest observed value and highest predicted value over all hours and monitoring stations. An acceptable range of ± 15-20 percent is specified.

Normalized bias - This test measures the model's ability to replicate observed patterns during the times of day when available monitoring and modeled data are most likely to represent similar spatial scales. An acceptable range of ± 5-15 percent is specified.

Gross error of all pairs greater than 60 ppb - This test compares the differences in absolute magnitude of the error between the observed and predicted concentrations over 60 ppb at specific points. In conjunction with bias measurements, this test provides an overall assessment of base case performance and can be interpreted as precision. An acceptable range of 30-35 percent is specified.

Further, the Guideline recommends the following graphical displays to be analyzed:

Time-series plots - These plots depict the predicted and observed hourly ozone values for each for each monitoring station. The time-series plots assist in evaluating the model's ability to reproduce the peak prediction, the presence of any significant bias within the diurnal cycle, and the timing of the predicted and observed ozone maxima.

Ground level isopleths - Ground level isopleths display the spatial distribution of predicted concentrations in relation to observed values. The isopleths provide information on the magnitude and location of predicted pollutant "plumes". Superimposing observed hourly or daily maximum concentrations on the predicted isopleths reveals information on the spatial alignment of predicted and observed plumes. Sub-regional biases of predictions versus observations may result from spatial misalignments.

Scatterplots of predictions and observations - Scatterplots depict the extent of bias and error in the ensemble of hourly predictionobservation pairs. Bias is indicated by the systematic positioning of data points above or below the perfect correlation line, whereas error is identified within the dispersion of points.

Quantile-quantile plots - These plots compare the frequency distribution of the observed and predicted concentrations. The observed concentrations are rank-ordered (sorted from highest to lowest concentration). The predicted concentrations are separately rank-ordered in a similar fashion. The observed and predicted values are then paired according to their rank and plotted on an x-y graph. This visually depicts any model bias over the frequency distribution. The closer the pairs approach a line with a slope of 1, the better the model numerically matches the set of observations. This statistic does not address the spatial accuracy of the predictions.

It is noted that additional statistical and graphical tests are strongly encouraged, and that the States committed to performing numerous additional analyses in the model evaluation protocol dated May 1992. This technical support document does not address these additional analyses.

EVALUATION

In evaluating the Basecase C modeling results for Episodes 1, 2, 3 and 4, all study days except one were within the USEPA's acceptable range for unpaired peak prediction accuracy. The one day that fell out of the range, June 27th from Episode 1, modeled a peak value 27.7% over the monitored peak for the day. However, the modeled peak was located over Lake Michigan, whereas the monitored peak of 118 ppb was measured along the Western Michigan shoreline. Because of the limitations of monitoring over the lake, it is not certain that the day's observed surface ozone concentrations reflected the actual maximum domain-wide value. The aircraft measurements for that day over the lake appeared to confirm that a higher ozone concentration may have existed over the lake. Additional information regarding the boundary conditions for the episodes might also be informative to better understand this situation, it is specifically noted that this single discrepancy with USEPA's unpaired peak prediction accuracy criteria does not preclude model validation.

All days fell within the USEPA's acceptable ranges for normalized bias and gross error. Review of the model's time-series plots demonstrated a good temporal agreement with the monitors. Spatially, model performance was acceptable. The one exception, Episode 2, could be resolved through further consideration of the meteorological parameters. USEPA encourages the participants in the LMOS to continue to pursue the investigation into enhancements to the prognostic wind model (CALRAMS). Again, however, this disparity does not preclude model validation and use for regulatory purposes.

USEPA reviewed the UAM-V vs. UAM-IV comparison runs submitted within the October 1, 1994 performance evaluation. These runs were included to document and support the study's reliance on the UAM-V model with the UAM-IV photolysis rates instead of the UAM-V photolysis rates. UAM-V's lakeshore modeled concentrations were closer in numerical value and spatial agreement to the lakeshore monitored concentrations than were the UAM-IV's modeled concentrations. For this reason, as allowed for by USEPA guidance, the LMOS participants chose not to use the full UAM-IV model. Furthermore, the Basecase C results demonstrated that the UAM-V model with the UAM-IV photolysis rates showed very good agreement with the observations. Therefore, USEPA agrees that the Basecase C modeling using the UAM-V model with UAM-IV photolysis rates is acceptable.

Conclusion

USEPA finds that the Basecase C model, as discussed in the preceding pages, is performing in an acceptable manner and can be used for regulatory purposes. However, if changes to the model inputs occur in the future, those changes, as they affect the model, will need to be re-evaluated at that time.