United States
Environmental Protection
Agency

Atmospheric Sciences
Research Laboratory
Research Triangle Park NC 27711

Research and Development

EPA/600/S3-86/016 April 1986

EPA

Project Summary

Evaluation of the PEM-2 Using the 1982 Philadelphia Aerosol Field Study Data Base

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This report describes an evaluation of the Pollution Episodic Model Version 2 (PEM-2). The results of various statistical measures and graphical comparisons of model concentrations against measurements obtained from 29 days of the Philadelphia Aerosol Field Study are presented. The PEM-2 is an urban-scale plume model capable of predicting average ground-level concentrations and deposition fluxes of one or two gaseous pollutants or particulates at multiple receptors. The two pollutants may be nonreactive or chemically coupled through a first-order chemical transformation. Hourly meteorological data and emissions from 300 point and 289 area sources within the Philadelphia metropolitan area were used to calculate 12-h and 24-h average concentrations of fine and coarse total particulate mass, fine sulfate, and sulfur dioxide.

Statistical tests for evaluation of model performance include standard measures of difference and correlation between measurements and model estimates paired in time and space. The particulate species were simulated very closely; however, the results must be interpreted with caution due to the large contribution from the regional background concentration which far exceeded the local urban source contributions. Differences between modeled and observed concentrations are discussed, and the results are viewed in relation to a previous evaluation of the model.

This Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The Pollution Episodic Model Version 2 (PEM-2) is an urban-scale model designed to predict short-term ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants from multiple point and area sources. The effects of dry deposition, gravitational settling, and a first-order chemical transformation are explicitly accounted for in the model, if desired. PEM-2 computes the horizontal and vertical dispersion parameters for both point and area sources from Briggs' urban dispersion curves. Concentration computations from area sources are determined numerically for eight downwind receptor grid squares. Optional methods are also incorporated to consider new plume rise and penetration equations and to account for bouyancy-induced dispersion.

This report describes an evaluation of the PEM-2 model with data collected during the Environmental Protection Agency's Philadelphia Aerosol Field Study (PAFS). This intensive field program was conducted from 14 July to 14 August 1982 in Philadelphia, Pennsylvania. The primary purpose was to obtain detailed data sets on ambient surface concentrations of gaseous and particulate pollutants, emissions, and relevant meteorological parameters with adequate time and spatial resolution for the evaluation of short-term source and receptor models for a major urban area.

The goal of the evaluation was to pro-

vide an objective determination of the accuracy of the model when tested in an operational mode against a suitably extensive urban data base. The model performance was determined by comparing calculated average concentrations with corresponding observed values for the following pollutant species: fine particulate (FP) total mass, coarse particulate (CP) total mass, fine sulfate, and sulfur dioxide (SO_2). The FP size cut-off is 2.5 μm and the CP size range extends from 2.5 to 10 μm.

An integral part of the PAFS program was an air monitoring network consisting of six sites strategically located within the Philadelphia urban area. The concentrations of the above pollutants were sampled on a 12h basis with average daytime (6 AM — 6 PM) and average nighttime (6 PM — 6 PM) concentrations; except SO_2 was measured at hourly intervals. Meteorological data input to the model consisted of the hourly surface observations of wind speed and direction, and temperature from the National Weather Service Office at the Philadelphia International Airport. Morning and evening mixing heights were derived from high resolution temperature soundings made during the program. Hourly mixing heights were obtained by interpolation, and stability class was determined from the hourly surface observations.

Hourly emission inventories of the four modeled pollutants were specifically developed with 300 major point sources and 289 area sources. The area source grid consisted of 17x17 square cells being 2.5 km on a side. Mobile source and minor point source emissions were also prepared on the same grid system and merged with the area emissions in the evaluation.

Model Evaluation

The model was executed for the 29 days of the PAFS program. The model domain consisted of 32x32 cells with the southwest corner of the grid located at UTM coordinates 444.5 km north and 4380 km east in zone 18. The model cell size of 2.5 km coincided with the area source grid and the model domain encompassed the entire emissions inventory area. The model code was specially modified to allow for the input of hourly emissions and its capacity was increased to accommodate the 289 area sources. Otherwise, no further changes were made to the model's code.

The pollutant species were computed from two model runs. In Run I, SO_2 and fine sulfate concentrations were computed. The day and night transformation rates of SO_2 were set at 7% and 3% per hour, respectively. Daytime and nighttime deposition velocities for SO_2 were 3 and 2 cm/s, and 0.2 and 0.1 cm/s for fine sulfate, respectively. Settling velocities for both species were assumed to be zero. FP and CP total mass concentrations were modeled in Run II for each 12-h period. Day and night deposition velocities were 0.2 and 0.1 cm/s for FP, and 0.5 and 0.5 cm/s for CP, respectively. A settling velocity for CP was set at 0.25 cm/s. These values for the transformation rates, and deposition and settling velocities were based on typical values reported in the scientific literature for large roughness features approximated by urban surfaces.

The calculated 12-h average concentrations resulting from the various local emissions sources were added to their appropriate background values. The latter were determined as the lowest observed 12-h concentration at one of the outer four PAFS sites located upwind of the downtown area during the averaging period. However, the background for SO_2 was assumed to be zero. It is acknowledged that this determination of the background is somewhat subjective and limited due to the small number of upwind sites. Additionally, the background values were found to be a significant fraction of the total predicted concentration.

The statistical measures of difference and correlation between model and observed concentrations identified by the American Meteorological Society applicable to model evaluation and uncertainty were determined. The evaluation report contains complete tables of all statistical results and various graphical displays. In the following discussion, observed concentrations are denoted by O and predicted values are denoted by P. Averages were determined from the total number of pairs.

The results for FP total mass over the entire data set show a mean ratio (P/O) of 1.24 and mean bias (O — P) of -4.7 $\mu g/m^3$ indicating the model slightly over predicted observed values. A correlation coefficient of 0.75 indicates a relatively high correlation between predicted and observed FP total mass. There was little difference between daytime and nighttime statistical measures. The mean O and P concentrations were 29.8 and 34.5 $\mu g/m^3$, respectively.

The model evaluation statistics for CP total mass were a mean P/O of 1.29 and a mean bias of -0.84; however, a correlation coefficient of only 0.25 reveals a large amount of randomness in the model-observed pairs. The mean O and P values were 14.6 and 15.4 $\mu g.m^3$ compared to a mean absolute error of 5.7 $\mu g/m^3$, which indicates that PEM-2 determined CP total mass to within a factor of two. The local source contributions were more important for CP total mass (i.e. background was about twice as large on average) than for FP total mass; however, the background concentrations remained a decisive factor in the overall CP mass levels in the urban area.

The mean ratio of P/O for fine sulfate was 1.45, and the mean bias of -1.31 $\mu g/m^3$ reveals the model slightly overpredicts observations. The mean O and P concentrations were 9.8 and 11.2 $\mu g/m^3$, respectively. There was a relatively high correlation coefficient of 0.77 for both day and night. The background value of fine sulfate was also a significant part of the concentration levels in the urban area.

The hourly SO_2 measurements provide a demanding test for short-term models like PEM-2. Graphs of the diurnal variation of observed and predicted SO_2 concentrations revealed a greater overprediction by the model at night than during the day at the three sites closer to the central urban area where there are major area source emissions and surrounding major point sources. At the three sites on the periphery of the urban area where area emission are much smaller, the model underestimated concentrations during the day, but still overestimated SO_2 at night. For 12-h averaged values, the mean ratio of P/O was 1.51; however, the correlation coefficient was 0.1. The mean bias was -5.71 $\mu g/m^3$ which also indicates that the model overpredicted concentrations. The model performed better during the day than at night for the 12-h averaged results.

Due to the significant impact of the regional background values to the overall concentrations, a stepwise regression procedure was also performed to investigate their impact on the model evaluation. This regression method consisted of fitting a linear relation between observed and background values. The next step involved the observed concentration as the independent variable and the background and modeled concentrations as dependent variables. Residuals and correlation coefficients were determined for both stepwise relations for all pollutant species. The results of the regression analyses revealed an incremental improvement when including the modeled concentrations in the stepwise regression; however, the higher correlations and smaller errors were not statistically significant. The observed ground-level concentrations of fine sulfate, and FP and CP total mass were highly

related to the background level. In addition, estimates for background concentrations based on the observed concentrations upwind appears to be adequate.

Conclusions

This report describes an evaluation of the PEM-2 model with the PAFS data base. The model performance was tested by statistical comparisons of predicted concentrations against observed measurements for four pollutant species. For sulfate and fine particulate total mass, the values for the correlation coefficient and index of agreement were high, and a large part of the estimated error was unsystematic. For coarse particulate total mass, the evaluation statistics were not as good by comparison, and the larger systematic error suggests room for improvement. Overall, the model slightly overpredicted for the particulate species.

The overall high degree of model performance for the particulate species should also be interpreted with caution since the background concentrations, arising from the regional inflow, exceeded the urban source contributions. Ideally, the background values should be obtained from monitoring stations at the grid boundaries, farther from the source region being modeled. Nevertheless, the background particulate concentrations derived from observed suburban sites and by wind direction analysis for each 12-h averaging period seem appropriate.

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The complete report, entitled "Evaluation of the PEM-2 Using the 1982 Philadelphia Aerosol Field Study Data Base," (Order No. PB 86-167 921/AS; Cost: $16.95, subject to change) will be available only from:
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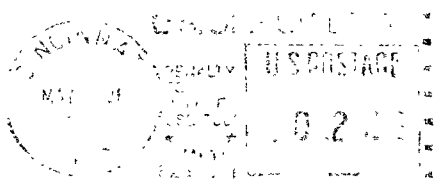

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