



Project Summary

Evaluation of the Pollution Episodic Model Using the RAPS Data

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The Pollution Episodic Model (PEM) is an urban-scale model capable of predicting short-term average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be nonreactive, or chemically coupled through a first-order chemical transformation. Up to 300 isolated point sources and 50 distributed area sources may be considered in the calculations. Concentration and deposition flux estimates are made using the hourly mean meteorological data. Up to a maximum of 24 hourly scenarios of meteorology may be included in an averaging period.

This report describes an evaluation of the PEM that used data from the St. Louis Regional Air Pollution Study (RAPS). This evaluation was designed to test the performance of the model by comparing its concentration estimates to the measured air quality data by using appropriate statistical measures. Twenty days, ten summer and ten winter, were selected from the RAPS data base for the PEM evaluation. The model's performance was judged by comparing the calculated 12-h average concentrations with the corresponding observed values for five pollutant species: SO₂, fine and coarse sulfates, and fine and coarse total mass. A first-order chemical transformation of SO₂ to fine sulfate was considered in the calculations in addition to the direct emission and dry deposition of all five pollutants.

For the twenty PEM evaluation days, PEM predicted average concentrations

of SO₂, and fine and coarse sulfates to within a factor of two. The model over-predicted the average concentrations of fine and coarse total mass by a factor of three to four over the evaluation period. This was attributed primarily to overestimation of emission rates and incorrect location of area sources, which dominate the fine and coarse total mass emission. Other possible sources of errors in the calculations are listed and discussed.

This Project Summary was developed by EPA's Environmental 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 (PEM) is an urban-scale model capable of predicting short-term ground-level concentrations and deposition fluxes of one or two gaseous or particulate reactive pollutants in an urban environment with multiple point and area sources. It is intended for studies of the atmospheric transport, transformation, and deposition of acidic, toxic, and other pollutants in urban areas to assess the impact of existing or new sources or source modifications on air quality, and for urban planning. The effects of dry deposition, sedimentation, and a first-order chemical transformation are explicitly accounted for in PEM.

This report describes an evaluation of the PEM that uses the St. Louis Reg-

ional Air Pollution Study (RAPS) data. This evaluation was designed to test the model's performance by comparing its concentration estimates to the measured air quality data by using several standard statistical measures of performance.

Twenty days, ten summer and ten winter, were selected from the RAPS data base for the PEM evaluation. The model's performance was judged by comparing the calculated average concentrations with the corresponding observed values for the following five pollutant species: SO₂, fine sulfate, coarse sulfate, fine total mass, and coarse total mass. In these species, the cut-off size between fine and coarse particle fractions was 2.5 μm. A first-order chemical transformation of SO₂ to fine sulfate was considered in the calculations in addition to the direct emission and dry deposition of all five pollutants.

Data Base

Twenty days, ten summer and ten winter, were selected from the RAPS data base by the U.S. Environmental Protection Agency (EPA) for the PEM evaluation. Detailed emission inventories of the RAPS region and meteorology and concentration measurements corresponding to these evaluation days were supplied by the EPA from the RAPS data base.

Hourly area and point source emission inventories for a typical winter day and a typical summer day for the St. Louis metropolitan area were supplied by the EPA on two magnetic tapes. The emission inventories were supplied on a numerical grid with a fixed origin at XUTM = 710 km and YUTM = 4250 km, which extended to 60 km in both x and y directions. The size of each emission grid cell for area sources was 5 x 5 km, thus giving 144 emission squares in the grid. Data tapes contained information on SO₂, sulfate, total particulate mass emissions, and the particle size derived from the 1976 RAPS Emission Inventory. An average conversion rate of 1.85% of SO₂ emissions was used to estimate the sulfate emission rates for both area and point sources from the known information on SO₂ emission, provided particulate emissions existed. In the case of point sources with no particulate emissions, but relatively large SO₂ emissions, the sulfate emissions were calculated on the assumption that in a short period of time, the conversion of SO₂ to SO₃ occurs and contributes to

the total mass in the region of interest. However, in the case of area sources, the SO₂ emissions were relatively small (3% of total SO₂ emissions); therefore, sulfate emissions could be neglected if there were no associated particulate emissions.

The size distributions of sulfate particle emissions from area and point sources were more difficult to estimate. Approximate base size distributions of sulfate for typical winter and summer days were determined. Based on other studies, about 50% of the sulfate was assigned to the size range less than 0.25 μm for the summer aerosol, and approximately 25% of the sulfate was assigned to this size range for winter aerosol. The base size distributions approximated were then used to estimate the sulfate size distributions in the area and point sources by relating the total particulate emissions (with associated size spectrum) from these sources to sulfate emissions.

Hourly measurements of wind speeds and directions, and temperatures from the 25 station Regional Air Monitoring System (RAMS) network were supplied by the EPA. Input files contained urban mixing heights, wind speeds and directions, atmospheric stability class, and temperatures: the input winds were RAMS network resultant winds. The stability classifications were supplied in the format required by PEM (i.e., stability classes 1-7).

Data tapes containing the observed gas concentration values from the RAMS network, corresponding to the twenty evaluation were provided. Separate files of high-volume and dichotomous sampler data were also provided. The data files were scanned for hourly average SO₂ concentrations, and 12-h average concentrations of total mass and total sulfur. The observed gaseous total sulfur concentrations were used to approximate SO₂ concentrations at the RAMS stations where the latter were not measured. The high-volume and dichotomous sampler data contained total sulfur and total particulate mass concentrations in μg/m³. The particulate data were further divided into fine and coarse categories based on a cut-off size of 2.5 μm. The total sulfur measurements were multiplied by a factor of three (the ratio of the molecular weight of SO₄ to the molecular weight of sulfur) to obtain the equivalent total sulfate concentrations.

Concentration measurements were not made at all of the 25 RAMS stations.

The observed SO₂ concentrations are 1-h average values. The total sulfur and total mass concentrations measured by eight out of the ten reporting RAMS stations were 12-h average values; only stations 103 and 105 recorded 6-h averages. To facilitate comparison with the model calculations, the observed concentrations of SO₂, fine and coarse sulfates, and fine and coarse total mass were converted into 12-h averages. This procedure gave two (12-h average) observed concentrations per day for each of the five pollutants.

Model Evaluation Results

PEM concentration predictions were evaluated against the measured concentrations for five pollutants: SO₂, fine particulate sulfate, coarse particulate sulfate, fine particulate total mass, and coarse particulate total mass. These five quantities were calculated in three model runs that used different sets of input data. It was assumed that SO₂ chemically transforms into fine sulfate at a constant rate, and there is no contribution to coarse sulfate concentrations from this transformation.

A chemical transformation rate of SO₂ to fine particulate sulfate of 5% per hour was used. This value was held constant throughout the model runs regardless of meteorological and other conditions.

Deposition (V_d) and gravitational settling (W) velocities were varied depending on the pollutant in each model run. For example, V_d was 2.0 cm/s and W was assumed to be zero for SO₂. No attempt was made to vary them by the atmospheric stability class or other meteorological conditions.

PEM uses a fixed calculation and receptor grid system. A grid system was designed such that PEM receptors either matched or formed a grid around the actual RAMS network stations. For point comparisons with the RAMS network stations, the four receptors in the grid squares around the RAMS station were summed and their average was assigned to the RAMS station location.

The numbers of point sources in this evaluation were 286 in winter and 275 in summer, thus nearly utilizing the maximum capacity of the model of 300 point sources. For point source calculations in this evaluation, a modification was made to the PEM program such that concentrations were calculated only for the receptors surrounding each RAMS station and not at the rest of the receptors. This required calculation of

only 84 out of a total of 2500 receptors. The model performance was evaluated by using several statistical measures. Two general measures of performance were used here: a) measures of difference, which included bias, variance, gross variability or root mean squared error (RMSE), and average absolute gross error; b) measures of correlation paired in space and time.

The ratio of the calculated (P) and observed (O) means for SO₂, P/O, was 1.24, and the ratio of the corresponding standard deviations was 1.12. However, the correlation coefficient was only 0.23 over the compared range (6.5 – 250 μg/m³) of concentrations. This suggests a large degree of randomness in the individual case-by-case comparisons of SO₂ concentrations. The differences D_i between observed and calculated SO₂ concentrations showed a clear bias for PEM to overpredict observed concentrations less than 75 μg/m³ and underpredict observed concentrations greater than about 125 μg/m³. The bias D over the entire evaluated range of SO₂ concentrations was -12.8 μg/m³. Thus, PEM was conservative, with a tendency to slightly overpredict the average SO₂ concentrations. The average absolute gross error |D̄| was 48.5 μg/m³, which was less than the mean of observed concentrations. Therefore, on the average, PEM predictions are within a factor of two of the observed SO₂ concentrations.

For fine sulfate concentrations, P/O was 1.1 and the ratio of the corresponding standard deviations was 1.2. The correlation coefficient was 0.41 over the compared range (1 to 30 μg/m³) of the concentrations. The model tended to overpredict O_i < 18 μg/m³ and underpredict O_i > 20 μg/m³. The bias D̄ over the entire range of concentrations was -1.0 μg/m³, (i.e., the model is slightly conservative). The average absolute gross error |D̄| was 4.8 μg/m³, which was much less than the mean of observed concentrations. Therefore, averaged over the entire data base, PEM calculations of fine sulfate concentrations were within a factor of two of the corresponding observed values.

Coarse sulfate (particle size ≥ 3 μm) concentrations from the model evaluation results for direct emissions of sources only were low (generally less than 3 μg/m³). The ratio of the means of calculated and observed values of concentrations, P/O, was 0.52, and the ratio of the corresponding standard deviations was 0.9. The correlation coefficient

was 0.38 over the compared range of concentrations. The model slightly underpredicted the concentrations, with a bias of D̄ = 0.5 μg/m³ and an average absolute gross error of 0.66 μg/m³. The latter was 59% of the mean of observed concentrations. Thus, on average, the calculated coarse sulfate concentrations were within about a factor of two of the corresponding observed values. The model performed somewhat better in winter than in summer.

The results clearly showed that PEM overpredicted fine total mass concentrations. The observed concentrations were less than 80 μg/m³, but the corresponding calculated values ranged up to 300 μg/m³. The larger calculated concentrations were generally associated with weak diffusion conditions characterized by strong stabilities, low wind speeds, and shallow mixing depths that were typical of several of the winter evaluation days. The ratio of the means, P/O, was 3.1 and the ratio of the corresponding standard deviations was 6.0. The model significantly overpredicted the concentration, with a bias of D̄ = -70.8 μg/m³ and an average absolute gross error of 72.1 μg/m³, which was 2.1 times the mean of observed concentrations. The model overpredicted concentrations at stations within the city by a factor of three or less, and accurately modeled the two outlying stations.

The model evaluation results for coarse total mass (particle size ≥ 3 μm) concentrations were qualitatively similar to those obtained for fine total mass evaluation.

Conclusions

This report described an evaluation of PEM that used twenty days of data from the St. Louis RAPS. This evaluation was designed to test the model performance by comparing its concentration estimates for five pollutants to the measured air quality data by using appropriate statistical measures of performance.

For the twenty evaluation days, PEM predicted average concentrations of SO₂ and fine and coarse sulfates to within a factor of two. The model overpredicted the average concentrations of fine and coarse total mass by a factor of three to four over the evaluation period. The significant differences between the calculated and observed total mass concentrations may be attributed to a number of reasons:

1. Hourly point and area source emission inventories were available for only one winter day and one summer day. These inventories were further averaged over two 12-h periods per day for use as input to PEM. Analysis of the emission inventories indicated a core of steady emission sources with various other area and point sources coming on or off line throughout the modeling period. Running PEM on an hour-by-hour basis might account for this variability of emissions but the modeling costs would be prohibitive. Despite this variability, both fine and coarse sulfates were predicted to within a factor of two for the total means as well as across the 12-h averaging period. However, the variability in emissions appears to be very important for fine and coarse total mass, because these emission rates were significantly larger and dominated by ground-level sources.
2. Point sources dominated the emissions of SO₂ and fine and coarse sulfates. Area sources dominated the emissions of fine and coarse total mass, and the sulfate components of fine and coarse total mass emissions from area sources were negligible compared to the nonsulfate components. The nonsulfate total mass consisted of fugitive dust, highway, residential, commercial, industrial, and other particulate emissions of different sizes that were difficult to estimate accurately. No information is available on the variability of these emissions. Any errors involved in the estimation and location of these sources would significantly affect the calculated concentrations due to the relatively large emissions from area sources.
3. Because of the 12-h averaging for periods 00-12 and 13-24 h, little can be said about the diurnal variation of model performance in this evaluation. There were also significant differences between the first and second averaging periods in the mean residuals of fine and coarse total mass. This may have been associated with the diurnal variability of area source emissions of these species and with errors in stability classification. The first 12-h averaging period was generally characterized by stable conditions, with weak diffusion conditions. Hence, the calculated concentrations and residuals were larger for this period.

4. Constant deposition and settling velocities and transformation rates were used throughout the 12-h averaging period. This ignores the dependence of these variables on meteorological conditions such as wind, humidity, and thermal stratification. Also, using one constant set of values for deposition and settling velocities to describe the broad particle size spectrum $\geq 3 \mu\text{m}$ may not accurately represent the behavior of particles of different sizes.
5. The wind speed and direction input to PEM were the RAMS network resultant values. These are approximations to real conditions. Errors in wind direction may cause the model to affect particular receptors that may be completely ignored in reality. An underestimation of the actual wind speed leads to overprediction of the calculated concentrations.

Additional effort should be directed toward an examination of the model's response to emission variability, stability classification, and area source emissions and location. Experience has shown that area sources are the primary determinant in modeling urban ground-level concentrations of nonsulfate particulate matter.

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The complete report, entitled "Evaluation of the Pollution Episodic Model Using the RAPS Data," (Order No PB 84-232 537; Cost. \$10.00, subject to change) will be available only from.

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