United States
Environmental Protection
Agency

Atmospheric Sciences
Research Laboratory
Research Triangle Park NC 27711

Research and Development

EPA/600/S8-85/028 Mar. 1986

EPA

Project Summary

Methods for Mesoscale Modeling for Materials Damage Assessment: User's Guide

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Assessment of acid deposition damage to materials requires, as a minimum, detailed knowledge of SO_2 (gas) and wet H^+ annual deposition fields on time and space scales consistent with the mechanisms of damage and the distribution of materials at risk. Methods for urban air quality SO_2 modeling are reviewed, and a set of simplified algorithms is presented suitable for relatively rapid assessment of a large number of cities. The method is relatively "meteorology free" in that regional wind roses have been incorporated into the parameterization rather than site-specific wind roses. Separate algorithms are presented for point and for area sources, and the model is designed to produce annual average concentration estimates over 5-km grids. The Parameterized Air Quality Model-Annual (PAQMAN) is designed to mimic the performance of the Climatological Dispersion Model (CDM). McElroy-Pooler dispersion coefficients are used for point sources; whereas Briggs' plume rise and Pasquill-Gifford dispersion coefficients are used for area sources. PAQMAN results correlated well with CDM calculations for the New Haven and Pittsburgh Metropolitan Statistical Areas (MSAs) with correlation coefficients of 0.90 and 0.80, respectively. Comparisons between PAQMAN and measured concentrations averaged over each MSA were also favorable over the entire spectrum of 112 MSAs.

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

One of the components of the National Acid Precipitation Assessment Program (NAPAP) deals with damage to materials in the environment. Such an assessment requires detailed information on deposition of corrosive agents, namely SO_2 and wet H^+, on spatial scales compatible with materials distributions in urban areas. The objective is to provide sufficiently accurate deposition estimates for materials damage for over 100 cities.

Since extant urban SO_2 monitoring data are inadequate to characterize the distribution of air quality within a city (i.e., monitors tend to be located only to meet specific regulatory needs), a modeling approach is necessary to estimate detailed annual average SO_2 concentrations. The basic approach used is a parameterization in which closed-form algorithms are developed for point and area sources; these algorithms mimic the performance of EPA's Climatological Dispersion Model (CDM) and allow rapid assessment of a large number of sources. The model, called PAQMAN, has been applied to over 100 MSAs in which materials distributions have been derived. The intent is that this methodology will serve as a useful sub-grid feature for mesoscale and regional scale models.

Objectives

The objectives of this study are to

(1) Develop an acceptable parameterization model for SO_2 that will allow the rapid assessment of a large number of sources using limited computer resources, and at the same time mimic the predictions of a more refined model with reasonable accuracy.

(2) Apply this parameterized model to several MSAs in order to accurately predict SO_2 distributions for urban areas.

(3) Develop data bases for regional SO_2 background (non-urban) concentrations that are consistent with the urban SO_2 observations, and for urban H^+ (wet) deposition.

Technical Approach

Since long-term annual average estimates of SO_2 are needed for the materials assessment, a steady state Gaussian model was considered appropriate as the baseline model to be used to develop PAQMAN. CDM was selected as the reference model because of its acceptance as a standard EPA regulatory model and its extensive previous application to urban areas.

Simplified calculation methods were developed from parametric studies of both point and area sources. For point sources, a range of stack heights and flue gas conditions was used; various geometric patterns and emission densities were used for area sources. Following the recommendations of EPA for urban areas,[1] the McElroy-Pooler dispersion coefficients were applied to area sources. Plume rise was calculated according to Briggs.[2] Three wind roses were used for the parametric studies: JFK Airport (New York), Pittsburgh, and Cincinnati. These were then collapsed into generic categories: "coastal" (JFK) and "interior" (a blend of Pittsburgh and Cincinnati), in order to eliminate site-specific wind roses in favor of regionally representative meteorology.

The point source calculation algorithms were based on the use of the average distance (r_{max}) from the source to the location of the maximum annual average ground-level concentration as a scaling parameter. This distance was found to be a function of stack height. The downwind ratio of concentration with respect to the maximum concentration was found to be a function of the ratio of downwind distance to the scale length, r_{max}. The maximum ground-level concentration (χ/Q) was found to be a function of stack height. These curve fits, shown schematically in Figure 1, represent the entire spectrum of point source dispersion patterns, which were averaged around the compass to remove site-specific wind direction effects. The method implies that all stack heights can be generalized into one representation, as demonstrated in Figure 2.

Emission density (Q/A) and scale length (grid size) were the controlling parameters for the area source calculation algorithm. The underlying assumption is that concentration patterns tend to "flow" from areas of high emission density into adjacent areas of lower emission density and that the opposite effect is negligible. This was deduced from parametric calculations with CDM, using concentric squares of varying emission densities.

Calculated area source concentrations are sensitive to the scale length (emission grid size) applied to the emissions inventory. For example, as the size of the source diminishes at constant emission density, it approximates a point source of effectively zero strength. With increasing scale, on the other hand, larger absolute amounts of emissions become involved, which increase the spatial impact of the area source. While it may have been desirable to have the area scale length compatible with the materials inventory and land use elements (census tract level ~1 km^2), the parametric CDM runs revealed that a calculation grid of greater than 1 km was essential in order to achieve satisfactory computing times. A 5-km grid provided an acceptable compromise between spatial resolution and computing resources.

A rectangular grid (5-km spacing) was overlaid that encompassed the census tract centroids within each MSA. All sources inside this grid were included in

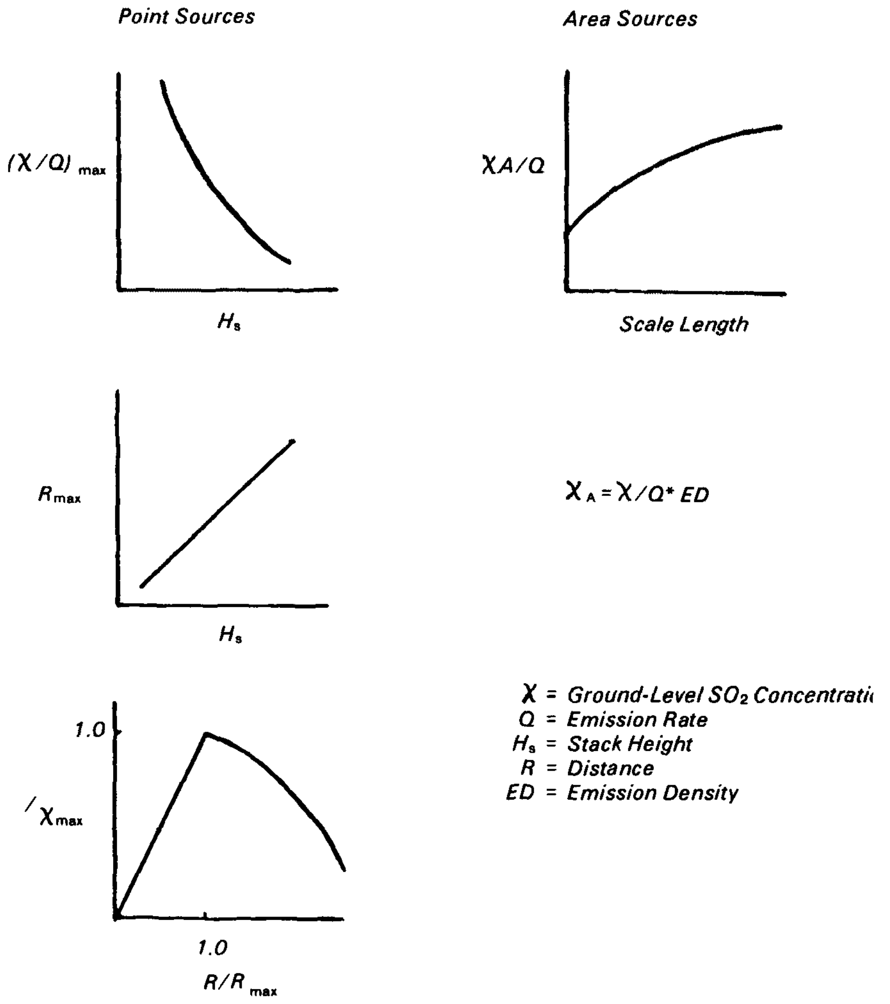

Figure 1. *PAQMAN point and area source algorithms.*

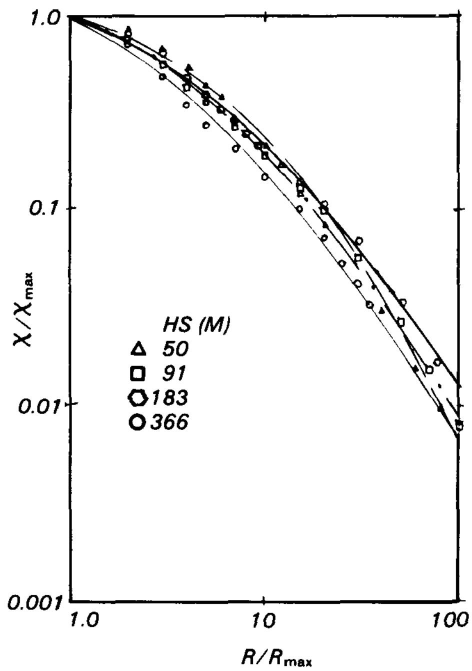

Figure 2. Concentration ratio vs. distance ratio CVG wind rose—varying H_s McElroy-Pooler σ's.

the model calculations. Sources with stack heights less than or equal to 62 m were grouped and treated as area sources; those with stack heights greater than 60 m were treated as point sources in the model. In addition, all stack heights <19 m were set to 19 m, assuming that they were located atop buildings. Sources within 50 km outside of the grid boundaries were all treated as point sources, but were retained only if their concentration at the nearest grid cell centroid exceeded 0.1 μg/m³. This procedure was very effective in eliminating unnecessary calculations, which reduced computer time substantially. In addition, the emissions from groups of sources located within 0.1 km of each other were aggregated, and a weighted average stack height was used in the calculation algorithms. While this procedure tends to overestimate the combined concentration if the stack heights in the groups differ greatly, it prevents groups of small sources from being overlooked because each is too small.

Emissions data were obtained from the NAPAP emissions inventory (Version 2.0) for 1980. In addition, emissions due to residential space heating (oil fuel) were derived on the census tract level and summed within each grid square. These oil-heat emissions were combined with the NAPAP area source emissions (stack heights ≤62 m) for each grid square. A check on potential problems with the emissions inventory was implemented by listing all sources that contributed to a calculated SO_2 concentration above the primary air quality standard of 80 μg/m³. This allowed spot checks for erroneously calculated low stacks or high emissions and identified gross underestimates of ambient concentrations (missing sources or erroneously high stacks).

In many cases, regional background is an important portion of the total observed concentration. Estimates of these background concentrations were provided by Dr. Jack Shannon of Argonne National Laboratory who used the ASTRAP model[3] and 1980 NAPAP emissions data (Version 2.0). Urban wet H^+ concentration for each MSA was interpolated from regional values from the Acid Deposition Systems (ADS). The rationale for this assumption was that neutralization of acidity effects from local urban SO_2 and NO_x emissions are neutralized to a certain extent by alkaline particles in urban dust.

Results

Comparison of PAQMAN with CDM Calculations

The CDM model was exercised in detail for two case study cities: New Haven, Connecticut; and Pittsburgh, Pennsylvania. Agreement between the actual CDM results and those from the simplified algorithms (PAQMAN) were quite good, as shown in Figures 3 and 4. Correlation coefficients were 0.90 and 0.80 for CDM and PAQMAN, respectively. For both cities, the highest concentrations were due to area sources, for which the two models agree very well. The scatter in data at the lower-to-middle concentration levels, in general, reflect our decision to ignore wind direction effects in favor of averaging. Since Pittsburgh has major point sources to the east of the MSA, PAQMAN SO_2 concentrations tend to be over-predicted with respect to CDM because the prevailing winds are westerly. In contrast, New Haven is affected by major point sources to its southwest; therefore, PAQMAN under-predicts relative to CDM for the same reason. It is hoped that, in general, this effect will balance and produce no net bias in the overall assessment of all 112 MSAs.

Comparison with Monitoring Data

A comparison of both model calculations with ambient measurements is shown in Figure 5 for Pittsburgh (selected because of its extensive monitoring network). The two models showed excellent agreement with ambient measurements, including the background SO_2 estimate from ASTRAP.

Figure 6 compares the predicted concentrations from PAQMAN averaged over the entire grid versus the average observed concentration for the MSAs. Overall, the model performed very well (slope is 0.81 ± 0.06) considering that

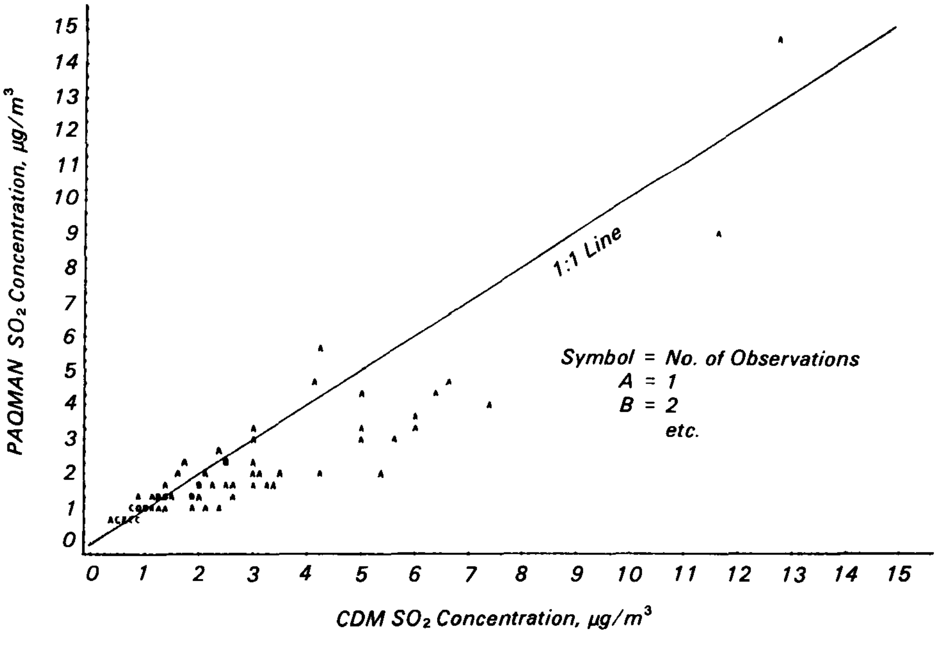

Figure 3. Comparison of PAQMAN and CDM SO_2 concentration estimates for New Haven.

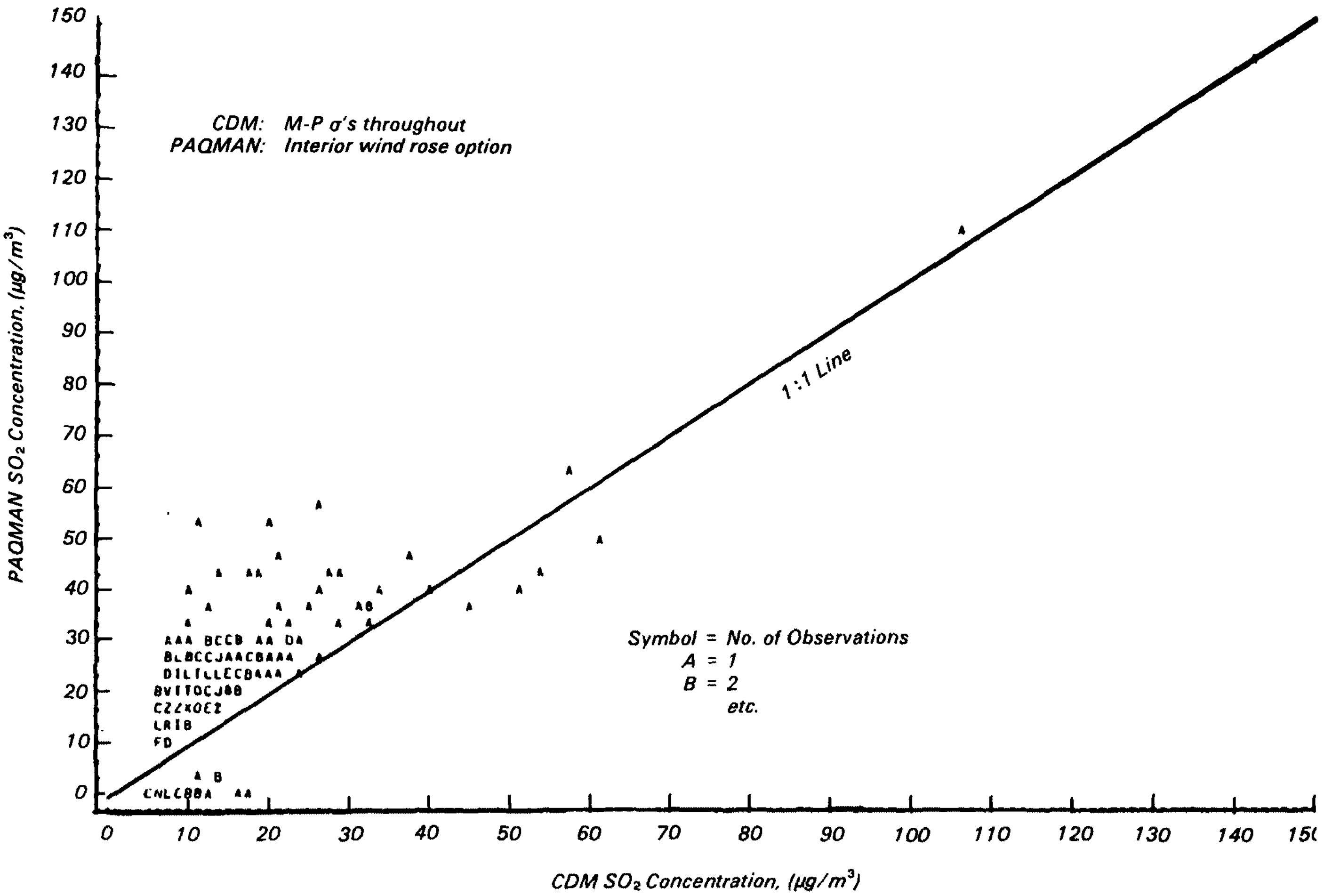

Figure 4. *Comparison of PAQMAN and CDM SO_2 concentration estimates for Pittsburgh.*

monitored data may not necessarily be representative of the entire urban center. Many of the higher concentrations (maximum concentrations, not shown) predicted by PAQMAN resulted from clusters of sources very close to each other (industrial complexes in cities such as Baltimore, Gary-Hammond, Cleveland) that fall into the same grid square. Downwash, a frequent feature of such complexes with short-to-moderate stack heights, can lead to very high concentrations. In most cases, the maximum concentration thus estimated would occur on plant property, which in a regulatory sense, is not classified as "ambient air." Therefore, monitoring data are not required and are in fact non-existent in most cases.

Discussion

The underlying assumptions of this methodology are that all stack heights can be generalized into a single representation and that local meterorology over a long-term (annual) basis can be generalized into a regional representation. These assumptions for the most part will not introduce any net bias for a large number of sources scattered "evenly" around an urban center, but are not applicable to isolated source assessments. The tendency toward over- or under-prediction for MSAs in which sources are more concentrated in one section than another (New Haven and Pittsburgh) suggests that wind directional effects may have to be incorporated in some way within these algorithms. Furthermore, additional algorithms for other meteorological regions (Great Lakes, interior Mid-West, interior East, etc.) may have to be develped.

The calculations for the 112 MSAs reveal that despite some high predicted concentrations, average annual SO_2 levels within the urban areas are low (20-30 µg/m³). This indicates that the urban contribution, in terms of SO_2, is comparable to that contributed by background levels, on the average. In terms o damage assessment, these findings imply that the sources outside of the city ar just as important as local sources.

Conclusions

The following were concluded fro this study.

1. A set of simplified algorithms tha mimics the CDM model and i suitable for rapid estimation of SO distributions for urban areas (MSAs has been developed. Test-cas studies have shown that the parameterization model (PAQMAN provides reasonable representation of CDM calculations (accurac estimates are about ±25%), especially for the higher SO_2 levels Both models were shown to compare favorably with monitorin data.
2. PAQMAN predictions for 11 MSAs indicated that annual aver

age SO2 levels that were averaged over the urban areas were comparable to background levels, which sugests that a considerable part of the materials damage costs in urban centers comes from pollution from outlying areas.

3. The results also reveal some problems in the model that need to be examined further, such as sensitivity of prediction to the assignment of sources as either point or area sources, based on stack height; the incorporation of methodology to deal with wind direction effects as well as additional regional meteorological regimes; and methods to estimate urban H^+ concentrations.

References

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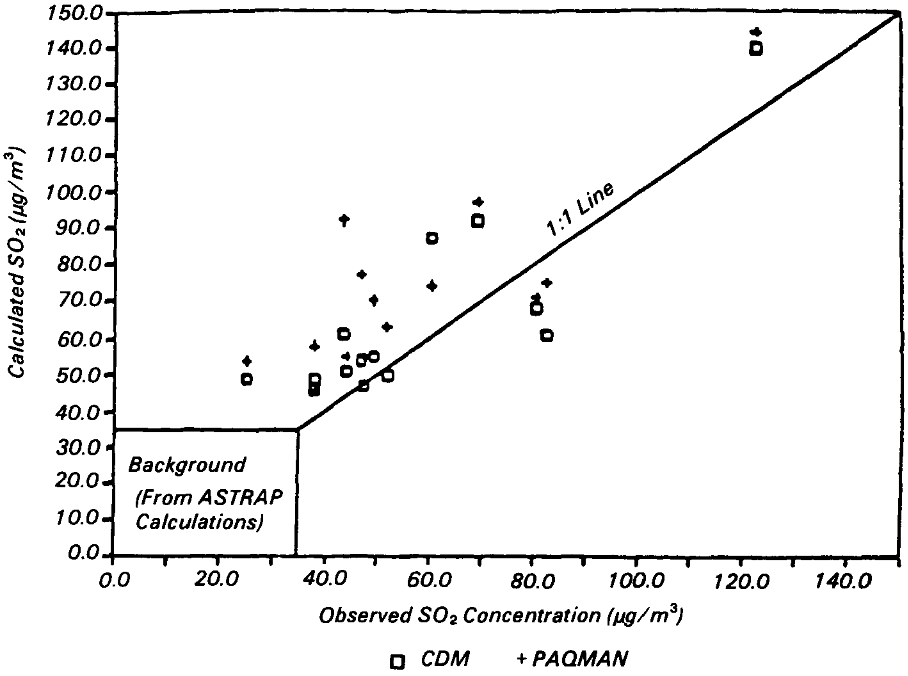

Figure 5. Calculated vs. measured SO_2 for Pittsburgh.

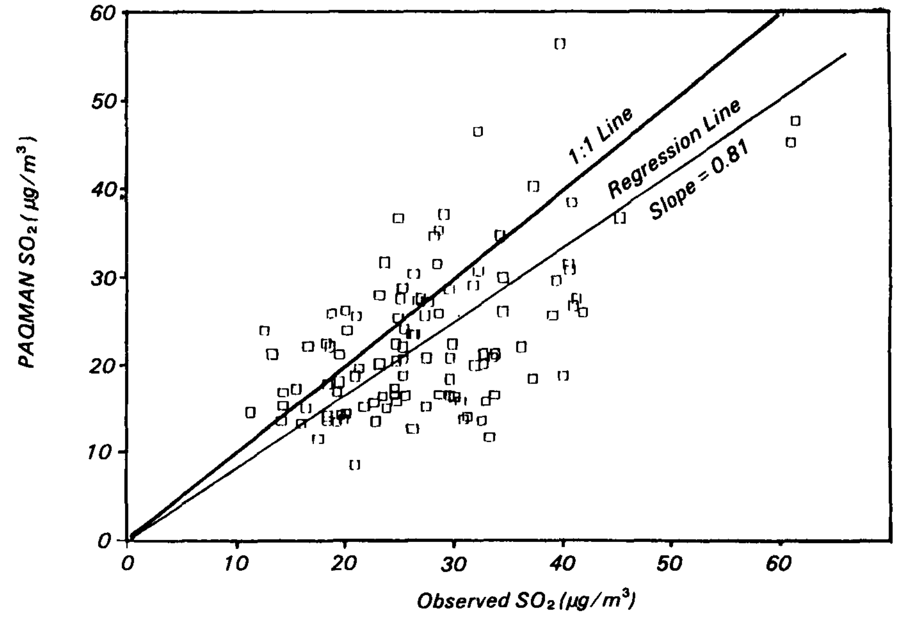

Figure 6. Comparison of average PAQMAN and average observed SO_2 concentration for 112 MSA's.

☆U. S. GOVERNMENT PRINTING OFFICE:1986/646-116/20784

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The complete report, entitled "Methods for Mesoscale Modeling for Materials Damage Assessment: User's Guide," (Order No. PB 86-144 862/AS; Cost: $11.95, subject to change) will be available only from:

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