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Project Summary

Air Quality Models Pertaining to Particulate Matter

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This report describes an evaluation of the Pollution Episodic Model, an urban-scale dispersion model that incorporates deposition, gravitational settling, and linear transformation processes into the predecessor model, the Texas Episodic Model. A sensitivity analysis of the model was performed, which included the effects of deposition, gravitational settling, and receptor grid size. Recommendations are made to improve the performance and flexibility of the model.

Pollution Episodic Model was applied to a source inventory of the Philadelphia area to provide a preliminary estimate of source apportionment. Pollution Episodic Model modeling employed both hypothetical and actual meteorology. Results indicate that area source emissions dominate total suspended particulate, sulfur dioxide, and sulfate concentrations at urban receptors. A large fraction of the inhalable particles may arrive from distant sources.

This report also contains an overview of receptor models (RMs) used for the source apportionment of aerosols. Some diagnostic procedures for RMs are evaluated with a synthetic data set. Described are receptor model tradeoffs and protocols and possible hybrid dispersion/receptor models. Issues regarding the intercomparison of source apportionments from receptor and dispersion models are highlighted with reference to the 1982 Philadelphia study.

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 principal objective of this work was to assess the two fundamental approaches to source apportionment of aerosol concentrations: source-oriented dispersion modeling (DM) and receptor modeling (RM). We aimed to define the strengths, limitations, areas of applicability, and possible protocols for the use of these methods in the regulatory context. The specific objectives included the following:

(1) Assessment of the new Pollution Episodic Model (PEM), a dispersion model that incorporates deposition, settling and transformation processes into the standard Gaussian plume dispersion algorithm. Pollution Episodic Model is an extension of the Texas Episodic Model (TEM-8). This report contains a discussion of the verification, applicability, and limitations of PEM. Suggestions are given to improve the versatility of the model.

(2) Review and general comments about receptor models. Part of this project involved a review of the models and literature that make up the current understanding of receptor techniques, as well as our experience with receptor models and similar statistical problems. The current status and capabilities of RM are discussed, with attention to the potential uses of RM in the regulatory process and the

application of diagnostic tools to RM that might be part of the modeling protocol.

(3) Discussion of potential hybrid dispersion-receptor models. There are a number of ways to combine source and receptor models. Currently, it is not clear that hybrid models are feasible and desirable. However, it is clear that contributions from each approach can be made to improve the other technique in certain circumstances. Recommendations are made regarding the development and application of hybrid models in intermodel comparisons.

(4) Comparison of DM and RM in the Philadelphia Study. In July and August of 1982, data were collected in the Philadelphia area, in part to compare source apportionments from DM and RM on the same, real data. Ground rules and certain specific tasks were required to make that comparison as meaningful as possible. Guidelines and a discussion of issues for this comparison are presented. Preliminary modeling results that used PEM and a source inventory compiled for the Philadelphia area are given.

Evaluation of the Pollution Episodic Model

The PEM model successfully incorporates simplified deposition, gravitational settling, and linear transformation processes. Pollution Episodic Model simultaneously calculates concentration and deposition over an urban-scale area in a rectangularly gridded receptor network.

With respect to deposition, PEM provides greater flexibility and some increased realism over comparable models. For example, the Industrial Source Code (ISC) model simulates gravitational settling by tilting the (normally horizontal) plume centerline; deposition is modeled by the partial reflection of the source contribution. Settling and deposition processes alter the distribution of mass within the plume. The ISC model's treatment is not altogether satisfactory because it does not model the modified distribution. Consequently, the ISC model tends to overpredict concentrations near the source and underpredict concentrations at large distances.

The PEM source code was checked for obvious errors or omissions. No mistakes were found. The source code was then compiled on the IBM FORTRAN V compiler. Only one "block data" per program is permissible with this compiler. The source code was modified accordingly.

The PEM was used with simple source and meteorological conditions in each stability category. Results were compared to the TEM-8 model. This showed good agreement, provided that the TEM time step was specified to be 10 minutes. Both models use the same P-G-T dispersion coefficients, but TEM increases these coefficients for calculating one hour averages. (The basic averaging period in PEM is one hour; in TEM, it's 10 minutes.) Maximum differences between the two models were under a few percentage points. However, under the most stable categories at relatively long downwind distances, maximum differences could range up to about 30 percent. These differences occurred because TEM uses "look-up" tables for dispersion coefficients at discrete distances, while PEM uses piece-wise approximations. Although both methods should be sufficiently accurate for model applications, the piece-wise approximations in PEM may provide more consistent results. Finally, analyses were performed to verify the model's response an sensitivity to changes in settling and deposition velocities, transformation rates, and area source treatment.

The PEM model was found to be easy to use (even without a user's guide). However, the versatility and convenience of the PEM program could be improved. Some of the recommendations in this section result from our experience with the model; others are proposed in view of expected applications. Implementation of the minor changes to the model (e.g., bookkeeping operations, additional outputs, and new user options) would facilitate sensitivity analysis and source apportionments. Other changes might increase the realism of the model. The somewhat increased complexity, memory storage, and computer time required by the model would not be important considerations to most model users.

Of the recommended changes, the most important improvements that increase model credibility are those concerning area source modeling. For sulfate modeling, hourly variation of transformation rates and elimination of cutoff distances for point and area source calculations are the most relevant. For TSP modeling, source-specific specification of particle size or deposition and settling velocity are important. The development of a long-term version of PEM for seasonal or annual particulate concentrations would complement existing air quality models. Most of the remaining recommendations simply provide greater convenience for model users.

Receptor Models

Receptor models (RMs) are procedures that use observed aerosol characteristics to identify and quantify the sources of ambient air pollutants. The aerosol characteristics most frequently measured include chemical and elemental mass, optical properties, and particle size distribution. Less frequently measured characteristics include isotope ratios, organic and inorganic compounds, and crystalline structure. Unlike dispersion models, RMs do not require meteorological or source data. Source profiles may be used, but are not necessary.

In general, RMs use the following assumptions:

(1) The total aerosol mass at a receptor is a linear sum of the aerosol contributions from individual sources. In general, there cannot be any transformation of the aerosol from time of emissions at the source through atmospheric transport to collection and ultimate analysis.

(2) Characteristics of the aerosols are a linear sum of the aerosol characteristics from individual sources (e.g., elemental ratios are assumed to be constant between source and receptor).

(3) Source apportionment is possible only for those source classes that have identifying characteristics. No unique characteristic is needed, just a unique combination of characteristics.

(4) Chemical mass balance models require quantification of source characteristics (e.g., elemental ratios). Multivariate models require less precise descriptions, but patterns of characteristics must be recognizable. Sources with unknown or highly variable characteristics may not be distinguishable.

(5) For regression models, the number of characteristics must exceed the number of source classes, and errors (residuals) should be normally distributed and uncorrelated. For multivariate models, the number of filters must be sufficient for the degrees of freedom required for the number of filter characteristics and sources used

Deviations from these assumptions will degrade the validity of the receptor model. The magnitude of the deviations that typially occur in RM applications is not known at the present time. Also unknown is the susceptibility of RMs to such deviations. There are obvious situations where assumptions are violated and RM applications may not be useful.

Hybrid Approaches

There are several possibilities for hybrid dispersion/receptor models. Hybrid models use a receptor model approach in conjunction with source emission rates, source locations, and/or dispersion information. Such models conceivably might provide a more accurate and flexible means of source apportionment. They may also help reconcile differences between source and receptor models. All data, including meteorology, source emissions and profiles, and filter characteristics are used in coupled models. Coupled models intimately combine receptor and dispersion approaches, and thus may be the most complicated of the hybrid approaches. Coupled models might be classified by their primary orientation, around either dispersion or receptor approaches. For receptor-oriented hybrid models, outputs of DMs might be treated stochastically. Chemical Mass Balance (CMB) RMs might then be extended by either including DM predictions as priors in Bayesian optimizations, or by using DM predictions of source contributions as coefficient weights in weighted optimizations. Analogous methods are possible for multivariate RMs Here, preprocessed meteorological data might become new variables in a factor analysis or multiple regression model. Association of particular meteorological patterns with source class signatures may identify the likely direction and distance of contributing sources. Alternately, source contributions predicted by DMs may become variables in factor analyses, along with the usual filter characteristics. Associations of predicted source contributions with the respective source profiles may indicate areas of agreement between the models.

The second general type of coupled model is based around dispersion modeling. The (deterministic) inputs or parameters of DMs are considered as stochastic variables (with estimated distributions). Optimization is used to match DM predictions to observed concentrations or receptor-determined apportionments, at the same time maximizing the probability of the stochastic variables in the DM.

Some major issues can be identified relative to the use of receptor models. Currently, there is a substantial amount of imposed "intelligence" that is introduced into RM procedures by experienced practitioners. Present RM studies are generally custom-designed, including selection of source signatures, filters, and analysis. In the regulatory context, some of the discretionary elements of RM might have to be removed to reduce the chances for misuses of the models.

The variation in source profiles (over time and space) and the deviation from the RM assumptions can be determined from source or near-field measurements, or perhaps derived by using wind trajectory analysis. Synthetic data sets with realistic error structures and compositions for various aerosol regimes (e.g., rural western vs. urban eastern) may be used to construct RM protocols.

Hybrid models require more data than either approach alone Such models may be cost-effective if source inventories and meteorological data are available. If hybrid models permit significantly improved performance in terms of accuracy and flexibility of source apportionment, their expense and complexity may be justified in other circumstances. At present, hybrid models have not been demonstrated and critically evaluated.

Conclusions and Recommendations

A new dispersion model, the Pollution Episodic Model (PEM) was found to successfully incorporate deposition, gravitational settling, and linear transformation processes to the predecessor model, the Texas Episodic Model. Thus, PEM should permit greater realism in urban scale modeling. However, some improvements to area source calculations seem warranted.

Application of PEM to a source inventory for the Philadelphia area and a sensitivity analysis indicated the following:

(1) Area source emissions may dominate TSP, sulfur dioxide and sulfate concentrations at receptors located within an urban scale. Therefore, source inventory data for area sources, including source strengths, operating schedules, microinventories (around receptor sites), and the degree and method of aggregation of small sources may be critical to accurate dispersion modeling. Distant sources warrant less attention.

(2) A large fraction of the observed inhalable particle mass, particularly sulfate, probably comes from medium- and long-range transport and not from local sources. Preliminary modeling has shown that sulfate contributions from local sources are generally only a few micrograms per cubic meter, compared with measured values which average about 24 $\mu g/m^3$. However, the model examined a relatively short period, and the source inventory is known to be very approximate.

(3) Particle and gaseous concentrations from middle to far field sources (greater than 10 km) may be sensitive to deposition velocities, with greater effects at larger distances. For these sources, gravitational settling is relatively unimportant. Gravitational settling may be important only for sources located in the vicinity of monitors that emit large particles with high settling velocities.

(4) Sulfate concentrations from distant sources are sensitive to transformation rate, especially at low wind speeds.

Our review of the literature and experience with receptor models indicated the following:

(1) The temporal and spatial variation of source profiles, and the sensitivity of estimated apportionment to such variation is largely unknown. The amount of data needed for representative and useful results is also poorly defined.

(2) Generally, RM studies have been custom-designed, including selection of sources signatures, filters and analysis. A high degree

of subjectivity may be involved in the interpretation and use of data and models.

(3) Each type of receptor model is prone to certain failures and limitations. Chemical mass balance RMs are subject to problems of collinearity and influential points. Diagnostic procedurés can be used to determine whether these problems exist; remedial procedures may be able to minimize their effects. Standardized protocols may be required to ensure meaningful results and promote appropriate uses of RMs.

Both dispersion and receptor models have useful attributes for the source apportionment of aerosols. Dispersion models are predictive and diagnostic. Receptor models are primarily interpretive. Standardized uses of receptor approaches are possible; however, their applicability and limitations need to be defined.

Hybrid models, which combine aspects from both dispersion and receptor approaches, may have applications to many air pollution problems, including apportionment of ambient concentrations of criteria and hazardous pollutants, visibility impairment, and acid deposition. However, at present, hybrid models are poorly developed and defined. The development and validation of hybrid models will require an extensive data set for various conditions and localities.

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The complete report, entitled "Air Quality Models Pertaining to Particulate Matter," (Order No. PB 84-210 939; Cost: $11.50, subject to change) will be available only from:
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