United States
Environmental Protection
Agency

Research and Development

Atmospheric Sciences
Research Laboratory
Research Triangle Park, NC 27711

EPA/600/S3-88/008 Apr. 1988

EPA

Project Summary

Rocky Mountain Acid Deposition Model Assessment: Evaluation of Mesoscale Acid Deposition Models for Use in Complex Terrain

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The hybrid acid deposition/air quality modeling system for the Rocky Mountains makes use of a mesoscale meteorological model, which includes a new diagnostic wind model as a driver for a Lagrangian puff model that treats transport, dispersion, chemical transformation, and dry and wet deposition. Transport will be defined from the diagnostic wind model based on the wind at the puff center. The treatment of dispersion will be based on the parameterization in the PNL/MELSAR-POLUT, while retaining the MESOPUFF-II dispersion algorithms as an option. Based on the evaluation of the chemical mechanisms, the RIVAD chemistry appears to be the most scientifically sound as well as consistent with the Lagrangian puff model formulation. Treatment of dry deposition will use the CCADM dry deposition module with some minor adjustments. Wet deposition will be based on the scavenging coefficient approach, as used in the ERT/MESOPUFF-II.

This modeling approach was guided by the comments of members of the Western Acid Deposition Task Force (WADTF) given in a questionnaire mailed in August 1986 and at a meeting in May 1987 in Denver. The modeling approach recommended by members of the WADTF was use of a Lagrangian acid deposition model with a complex-terrain wind model to calculate long-term source-specific depos-ition of nitrogen and sulfur. This modeling approach had to be cost effective, simple enough for use by the regulatory agencies, and similar to models approved by the EPA for impact assessment. If possible, it was desirable that the model have the ability to calculate PSD increment consumption of SO_2 and TSP sources. The hybrid modeling system meets these requirements in the most technically rigorous manner possible, subject to the cost and complexity constraints. The modeling approach is not as comprehensive as the Eulerian model development effort (RADM) currently being carried out by the National Center for Atmospheric Research and State University of New Vork at Albany. However, this approach is more technically rigorous than those currently used by regulatory agencies, and will generate more defensible estimates of incremental impacts of acid deposition and concentrations in regions of complex terrain in the Rocky Mountains.

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

Acid deposition has recently become an increasing concern in the western United States. Although this problem may not be as acute in the western U.S. as it is in the eastern U.S., it is currently a concern of the public and regulatory agencies because of the high sensitivity of western lakes at high altitudes and the rapid industrial growth expected to occur in certain areas of the West. An example of such an area is the region known as the Overthrust Belt in southwestern Wyoming. Several planned energy-related projects, including natural gas sweetening plants and coal-fired power plants, may considerably increase emissions of acid precursors in northeastern Utah and northwestern Colorado and significantly affect ecosystems in the sensitive Rocky Mountain areas.

Under the 1977 Clean Air Act, the U.S. Environmental Protection Agency (EPA), along with other federal and state agencies, is mandated to preserve and protect air quality throughout the country. As part of the Prevention of Significant Deterioration (PSD) permitting processes, federal and state agencies are required to evaluate potential impacts of new emission sources. In particular, Section 165 of the Clean Air Act stipulates that, except in specially regulated instances, PSD increments shall not be exceeded and air quality-related values (AQRV's) shall not be adversely affected. Air-quality-related concerns range from near-source plume blight to regional-scale acid deposition problems. By law, the Federal Land Manager of Class I areas has a responsibility to protect air-quality-ralated values within those areas. New source permits cannot be issued by the EPA or the states when the Federal Manager concludes that adverse impacts on air quality or air-quality-related values will occur. EPA Region VIII contains some 40 Class I areas in the West, including two Indian reservations. Similar designation is being considered for several of the remaining 26 Indian reservations in the region. State and federal agencies, industries, and environmental groups in the West need accurate data concerning western source-receptor relationships.

To address this problem, EPA Region VIII needs to designate an air quality model to estimate mesoscale pollutant transport and deposition over the complex terrain of the Rocky Mountain region for transport distances ranging from several kilometers to several hundred kilometers. The EPA recognizes the uncertainties and limitations of currently available air quality models and the need for continued research and development of air quality models applicable over regions of complex terrain.

The primary objective of the Rocky Mountain Acid Deposition Model Assessment project is to assemble a mesoscale air quality model based primarily on models or model components currently available for use by federal and state agencies in the Rocky Mountain region. To develop criteria for model selection and evaluation, the EPA formed an atmospheric processes subgroup of the Western Atmospheric Deposition Task Force, referred to as WADTF/AP. This group comprises representatives from the National Park Service, U.S. Forest Service, EPA Region VIII, the National Oceanic and Atmospheric Administration, and other federal, state, and private organizations. The design of this new model was based on the comments from the ADTF, who desired a cost-effective Lagrangian model capable of calculating incremental, long-term acid deposition and short-term concentration impacts over mesoscale distances in complex terrain.

A mathematical modeling system for describing the various physical and chemical processes associated with acid deposition and air quality must consist of several modules. These modules describe such processes as wind transport, dispersion, plume rise, chemical transformation, and wet and dry deposition. Although the modeling system must be an integrated, internally consistent package, it can be conveniently divided into two distinct principal parts:

Simulation of meteorological processes

Simulation of pollutant transport, dispersion, chemical transformation, and deposition.

Procedure

Four mesoscale meteorological and acid deposition models were selected for possible use in constructing the new hybrid acid deposition/air quality modeling system for the Rocky Mountain region. The candidate mesoscale meteorological models were the California Institute of Technology Wind Model (CIT/WINDMOD), the Pacific Northwest Laboratory MELSAR-MET model (PNL/MELSAR-MET), the Los Alamos National Laboratory ATMOS1 model (LANL/ATMOS1), and the Systems Applications, Inc. Complex Terrain Wind Model (SAI/CTWM). The candidate acid deposition models were the Environmental Research and Technology MESOPUFF-II (ERT/MESOPUFF-II), the Pacific Northwest Laboratory MELSAR-POLUT model (PNL/MELSAR-POLUT), the Systems Application, Inc. Regional Impact on Visibility and Deposition model (SAI/RIVAD), and the Systems Application, Inc. Comprehensive Chemistry and Acid Deposition Model (SAI/CCADM).

The candidate models were evaluated to determine which models best describe the complex processes that lead to acid deposition and air quality impacts in the complex terrain region of the Rocky Mountains and yet are consistent with the modeling approach desired by the potential users. The potential users requested a modeling approach that uses a diagnostic wind model as a driver for a Lagrangian acid deposition model. The resultant hybrid modeling system must be computationally efficient so that annual acid deposition impacts can be easily obtained and run on smaller computer systems.

Evaluation of the candidate wind models consisted of separate simulations using an idealized terrain obstacle (a bell-shaped mountain) and terrain from the Rocky Mountains. Based on these results a new diagnostic wind model (the DWM) was developed and further evaluated using the same tests as the candidate wind models and then comparing the results generated by the DWM with observations from the Rocky Mountains. The flexibility and adaptability of the new DWM was further evaluated by separate simulations in a complex terrain/coastal environment and within a large valley.

The evaluation of the candidate acid deposition models was accomplished by comparing how each of the candidate models treats the major processes that lead to acid deposition; transport, dispersion, chemical transformation, and dry and wet deposition. Based on this evaluation a new hybrid Lagrangian acid deposition model was constructed using the most technically rigorous components that were internally consistent with the over all framework of the hybrid modeling system.

Results and Discussion

Evaluation of the Mesoscale Meteorological Models

As an initial test, the four candidate mesoscale meteorological models were exercised using a three-dimensional bell-shaped mountain at a scale typically found in the Rocky Mountains and a complex terrain region in the Rocky Mountains using an initial uniform flow field. The results indicated that although the CIT wind model can treat the kinematic effects of terrain, it lacks Froude number flow adjustments (dividing streamline concept) and thus cannot simulate blocking effects if they are not defined by the input data. The CIT wind fields were minimally perturbed by the terrain.

The MELSAR-MET model was specifically designed to simulate blocking and deflection of air flows typically found in the Rocky Mountains under weak synoptic conditions. However, due to the model's unique interpolation scheme used to define gridded wind fields, spurious results are produced near the boundaries of the modeling domain. The MELSAR-MET wind fields also were not greatly perturbed from the initial uniform flow but did exhibit more terrain effects than the CIT model. The ATMOS1 model lacks a Froude number adjustment term to treat blocking and deflection but can provide a gross simulation of blocking through a region-wide stability dependent input parameter. The ATMOS1 model exhibited a large deflection of its air flows due to the terrain. The CTWM alone of the candidate meteorological models is designed to generate wind fields using only a domain mean wind as input. It is also the only model that can simulate upslope and downslope thermally generated flows. However, the CTWM is also the only candidate model that is formulated in a Cartesian coordinate system.

Use of a Cartesian coordinate system to simulate air flows in complex terrain is undesirable because air flows tend to follow terrain and increased vertical resolution is needed near the surface to resolve the terrain features. The problems with converting the CTWM to a terrain-following coordinate system were sufficient to eliminate the model from further consideration as a candidate. A comparison of the computation time required for the idealized test showed that the MELSAR-MET required the least computer time of the candidate models. The CIT wind model, the CTWM model, and the ATMOS1 model took approximately 4, 6, and 7 times the computer time that MELSAR-MET required.

Design of a Mesoscale Meteorological Model for the Rocky Mountains

The evaluation of the candidate mesoscale meteorological models indicated that no one of the candidate models was significantly superior over the others. Thus it was decided to construct a new diagnostic wind model (the DWM) using the best components from the candidate meteorological models. This wind model would utilize all existing wind observations while simulating the effects of complex terrain in regions with sparse observational data. The generation of the wind field by the DWM is accomplished in two steps. Step 1 is largely based on the approach used by the SAI/CTWM but formulated in a terrain-following coordinate system. The domain-mean wind for the modeling region is adjusted for the kinematic effects of terrain, thermdodynamically generated slope flows, and blocking effects. Step I produces a spatially varying gridded field of u and v wind components at several vertical levels.

Step 2 involves the incorporation of wind observations into the wind fields generated by step 1. An objective analysis scheme is used to produce a new gridded wind field. The scheme is designed so that the observations are weighted heavily in subregions where they are deemed representative of the mesoscale air flow, whereas in subregions where observations are deemed unrepresentative, the wind values produced by step 1 are weighted heavily. Once the new gridded wind field is generated, the vertical velocity out of the top of the modeling domain can be minimized.

In addition to wind fields, an acid deposition/air quality model requires other meteorological inputs, including boundary layer heights, temperatures, relative humidities, stability, precipitation, and other micrometeorological variables such as friction velocity and Monin-Obukhov length. The only candidate meteorological model that also generates fields of some of these meteorological variables is the MELSAR-MET model. The MELSAR-MET was designed specifically for the western Rocky Mountains and was written in a highly modular fashion, which allows for easy addition, replacement, or modification of any module. Thus the mesoscale meteorological model for the hybrid acid deposition model for the Rocky Mountains makes use of the MELSAR-MET framework, with the new DWM as its wind field generator.

Evaluation of the New Diagnostic Wind Model (DWM)

As for the candidate wind models, the DWM was exercised for the idealized bell-shaped mountain and the terrain from the Rocky Mountains using an initial uniform flow field. The DWM was exercised with its upslope and downslope parameterizations. These results produced wind fields consistent with the expectations for upslope and downslope flow regimes.

The DWM was then exercised for the Rocky Mountain terrain region using actual surface and upper-air meteorological observations. The DWM generated six vertical levels of gridded horizontal wind fields for each hour between 1600 on 17 September 1984 to 1500 on 18 September 1984. This period was selected because of the availability of three supplementary upper-air observations, in addition to the routine National Weather Service (NWS) surface and upper-air measurements, collected as part of the Atmospheric Studies in Complex Terrain (ASCOT) Brush Creek experiments. The Brush Creek experiments were designed to study drainage winds in the Brush Creek canyon. The formation of drainage winds generally requires clear, stagnant nights. If there is significant synoptic flow it will overpower the drainage winds.

The DWM was exercised twice for each hour of the 24-hour period, once using the routine NWS data only and once with the additional supplementary data. The DWM was thus evaluated qualitatively by comparing the wind fields generated with and without the supplemental data, and quantitatively by comparing the wind speeds and wind direction calculated in the simulation without the supplemental data and the supplemental observations themselves. A comparison of the wind speeds calculated by the DWM with the supplemental observations showed that the DWM underpredicted the wind speeds by 0.6 m/s out of an average observed wind speed of 2.1 m/s. The stagnant nature of the simulation period is confirmed by the fact that over 50 percent of the predicted and observed wind speeds at the supplemental data sites were calm. A comparison of the wind directions calculated by the DWM with the supplemental observations showed that the positive and negative deviations from the observed wind direction exactly cancel each other out, resulting in a net zero bias. Removal of the calm wind periods from the wind deviation distribution results in a much better match between the predicted and observed wind directions.

The new DWM was further evaluated by simulating two regions in California: a complex terrain/coastal region centered around Santa Barbara, and a region containing the southern California Central Valley and the Sierra Nevada mountains. For the complex terrain/coastal region, the DWM was exercised with up to 80 surface and 20 upper-air wind observation sites to produce hourly wind fields for 15 days. The DWM replicated the slope flows and sea breezes quite well. The flexibility of the formulation of the DWM was illustrated in the simulations within the Central Valley by using results from a two-dimensional simulation of a primitive equation model as input into the DWM. Again the DWM produced complicated nighttime downslope and daytime upslope flows.

Evaluation of the Candidate Acid Deposition Models

The candidate acid deposition/air quality simulation models were evaluated by comparing how each model treats the processes of transport, dispersion, chemical transformation, dry deposition, and wet deposition.

Transport. All of the candidate acid deposition models, except the CCADM, define transport by using the wind at the center of the Lagrangian plume or puff. The CCADM relies on user input for its trajectory definition. The sensitivity of trajectory definition to height above ground was examined by calculating air parcel trajectories at heights of 10, 300, and 1,000 m above ground, and four different release times using the DWM-generated wind fields from the Rocky Mountains. Results from the trajectory analysis can be summarized as follows:

The different transport characteristics between surface and elevated releases confirms the need for multilevel wind fields and the correct prescription of plume rise. Obtaining an upper-level wind by use of the power law relationship on the surface wind speed cannot accurately characterize transport in complex terrain,

When an emission release becomes well mixed, the advection of air parcels near the surface and parcels aloft should ideally be handled differently.

Dispersion. The candidate plume segment model, the RIVAD, and the two puff models, the MESOPUFF-II and MELSAR-POLUT, all use different parameterizations for defining the horizontal and vertical plume dispersion parameters, σ_y and σ_z. The CCADM requires user input for its diffusion and thus requires too much user interaction. The dispersion algorithms of the three models were evaluated by examining curves of the σ_y and σ_z at varying downwind distances and stability class (A-F) and comparing the curves with the usual Pasquill-Gifford-Turner (PGT) dispersion curves.

For unstable conditions the RIVAD produces the largest horizontal dispersion, while the MESOPUFF-II produced the best match with the PGT dispersion curves. For neutral conditions the RIVAD again produces the largest horizontal dispersion, while the MELSAR-POLUT algorithm that uses terrain roughness for neutral and stable conditions produced the next highest horizontal dispersion. For stable conditions the MELSAR-POLUT algorithms that uses terrain roughness produces the highest horizontal dispersion. This is not surprising since complex terrain enhances dispersion and the terrain roughness values used in these experiments were taken from terrain from the Rocky Mountains.

Chemical Transformation. Three of the candidate acid deposition models, MESOPUFF-II, RIVAD, and CCADM, contain chemical transformation modules. The MESOPUFF-II and RIVAD contain pseudo first-order chemical modules that describe the conversion of SO_4 to sulfates and NO_x to nitrates. The CCADM contains an explicit, comprehensive, highly nonlinear chemical kinetic mechanism that treats both gas- and aqueous-phase chemistry. Although the CCADM chemical mechanism is more detailed and technically sound than the pseudo first-order modules, the information required by the CCADM mechanism is not consistent with the desired formulation of the hybrid modeling system. Thus only the MESOPUFF-II and RIVAD psuedo first-order chemical mechanisms were evaluated.

The MESOPUFF-II chemical mechanism calculates the SO_2 and NO_x oxidation rates by statistically analyzing transformation rates produced by a complete photochemical mechanism over a wide range of environmental conditions. The RIVAD chemical mechanism uses a highly condensed chemical mechanism that uses the environmental conditions to estimate the hydroxyl radical, which is the principal oxidizer of SO_2 and NO_x in the gas phase. These two mechanisms were evaluated by comparing the responses of their predicted SO_2 and NO_x oxidation rates to solar radiation, temperature, relative humidity, and ozone, NO_x, and SO_2 concentrations.

The oxidation rates as calculated by MESOPUFF-II and RIVAD respond similarly to changes in solar radiation, although the ratios of the peak SO_2 and NO_x oxidation rates calculated by RIVAD are more consistent with our current understanding of photochemistry. The RIVAD mechanism is sensitive to changes in temperature while the MESOPUFF-II mechanism does not vary at all. Both models respond differently to changes in relative humidity but do agree for relative humidities in the range of from 25 to 50 percent. Changes in background ozone concentration result in similar responses from the two mechanisms, with the MESOPUFF-II exhibiting the most sensitivity. When either SO_2 or NO_x concentrations are increased, the RIVAD mechanism exhibits the most realistic responses, owing to the competition between these two species for the hydroxyl radical.

Dry Deposition. Two of the candidate acid deposition models, the MESOPUFF-II and the CCADM, use the resistance approach for the parameterization of dry deposition; the RIVAD uses the deposition velocity concept, while the MELSAR-POLUT does not treat pollutant loss due to dry deposition. Since the resistance approach is considered more technically rigorous than the deposition velocity concept, it has been adopted for use in the new acid deposition model for the Rocky Mountain region.

The two dry deposition algorithms based on the resistance approach in the MESOPUFF-II and CCADM model were evaluated by examining their calculated dry deposition velocities for different species over several surface types and variations of meteorological parameters, and comparing these calculated dry deposition velocities with the ranges of measured values from the literature.

For SO_2 the MESOPUFF-II and CCADM dry deposition algorithms predicted similar dry deposition velocity that agreed with measured values reported in the literature over all surfaces and almost all meteorological conditions. The exception to this was under F stability at approximately 2.5 m/s, where the MESOPUFF-II produced an anomalously high SO_2 dry deposition velocity peak.

For sulfate, dry deposition velocities calculated by the MESOPUFF-II and CCADM again respond in a similar fashion to changes in environmental conditions. However, the MESOPUFF-II predicts dry deposition velocities for sulfate that are always less than 0.1 cm/s, while the CCADM numbers tend to peak at around 0.3 to 0.8 depending on the surface type.

The predicted dry deposition velocities for NO_x agree very closely with the ones for SO_2 except that the anomalous peak at F stability and 2.5 m/s calculated by MESOPUFF-II is absent. The NO_x dry deposition velocities calculated by MESOPUFF-II and CCADM generally agree over all types of surfaces except for water.

Nitric acid has a very high deposition rate compared to the other gases studied because of its high solubility. The MESOPUFF-II and CCADM agree remarkably well on their predictions of nitric acid dry deposition velocities. There are very few measurements of the dry deposition velocity for nitric acid, but the few there are agree with the models' predictions.

Wet Deposition. Only the MESOPUFF-II and RIVAD wet deposition algorithms were consistent with the desired modeling approach and thus were evaluated by comparing their predicted wet scavenging rates for several species at different precipitation rates. For SO_2 the response of the wet scavenging rates in the two models to changes in precipitation were similar, although the MESOPUFF-II rates were approximately twice those of the RIVAD.

Despite the differences in their formulations, the MESOPUFF-II and RIVAD produce remarkably similar scavenging rates for sulfates for a liquid hydrometer. The MESOPUFF-II predicts lower scavenging rates for a frozen hydrometer, reflecting the fact that it is difficult for the particles to become embedded into ice crystals except through the process of riming. The RIVAD model predicts a wet scavenging rate of 100 %/h for nitric acid and all precipitation rates studied. The MESOPUFF-II also predicts high wet scavenging rates for nitric acid, but requires a precipitation rate of 1 in/h to obtain a scavenging rate of 100 %/h.

Design of the Acid Deposition/Air Quality Model for the Rocky Mountains

The evaluation of the four candidate acid deposition/air quality models indicated that no one of these models is the best choice for calculating source-specific acid deposition impacts in the Rocky Mountain region. Thus a new Lagrangian Gaussian puff model was designed, making use of the best components from the candidate models.

Transport within this new puff model would be defined by the wind at the plume center from the DWM. The dispersion algorithm from the MELSAR-POLUT model has been implemented in the new model, although the MESO-PUFF-II dispersion algorithms have also been retained as an option. The RIVAD parameterization of chemical transformation appears to be superior to the mechanism in the MESOPUFF-II and is the recommended mechanism in the new model. However, the MESOPUFF-II chemical mechanism has also been implemented as an option. The CCADM and MESOPUFF-II dry deposition algorithms produced very similar results; the CCADM algorithm has been implemented because it is more similar to the algorithms currently used in the state-of-the-art scientific acid deposition models, the RADM and ADOM. Finally, because of its ability to parameterize wet scavenging rates for both liquid and frozen precipitation, the MESOPUFF-II wet deposition algorithms have been implemented.

Conclusions and Recommendations

A model for calculating incremental impacts of acid deposition and pollutant concentrations in the Rocky Mountains has been designed using the components from existing models that are scientifically sound and also internally consistent with the overall modeling approach. Before each component was inserted into the modeling system, it was thoroughly evaluated to assure its scientific accuracy. The hybrid modeling system was designed in a highly modular fashion so that when new modules describing atmospheric processes become available they can be easily integrated into the modeling system. The authors recognize the inherent uncertainties and limitations in all air quality simulation models.

☆U.S. GOVERNMENT PRINTING OFFICE: 1988/548-158/67104

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The complete report, entitled "Rocky Mountain Acid Deposition Model Assessment: Evaluation of Mesoscale Acid Deposition Models for Use in Complex Terrain," (Order No. PB 88-167 481/AS; Cost: $25.95, subject to change) will be available only from:
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