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Project Summary

Preliminary Evaluation Studies With the Regional Acid Deposition Model (RADM)

This summary focuses on the findings of preliminary evaluation studies of the National Center for Atmospheric Research (NCAR) Regional Acid Deposition Model (RADM). Current efforts in evaluating the gas-phase chemistry submodel have met with significant success, and an understanding of the smog chamber databases has been developed. Due to lack of adequate observation data, evaluation of aqueous-phase chemistry and dry deposition submodels has not been possible. The cloud process submodel is consistent with the available but small data set. Preliminary evaluation of the full RADM system using OSCAR (Oxidation and Scavenging Characteristics of April Rains) meteorology and wet chemical deposition data has achieved initial success, though it is far from conclusive. Much larger and extensive databases are required to test the system thoroughly. The meteorology driver for the RADM has shown considerable skill in forecasting the OSCAR IV meteorology. Simulations of sulfate and nitrate wet deposition for the first day of OSCAR IV are quite good. RADM-simulated three-dimensional chemical species distributions are consistent with preliminary data measured by NCAR under a separate program. The first test of RADM's capability for analyzing "what if" studies with hypothetical reductions in sulfur emissions is demonstrated. The findings confirm the complexity of directly observing potential benefit from emissions reductions.

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

A comprehensive Regional Acid Deposition Model (RADM) is being developed at the National Center for Atmospheric Research. The RADM is an evolving advanced Eulerian computer model simulating the processes and pathways related to acid deposition in eastern North America. The RADM system consists of a mesoscale meteorological model which drives a transport/deposition model containing modular descriptions of the gas-phase chemistry, cloud processes and aqueous-phase chemistry, and dry deposition.

The objectives for the RADM are threefold: (1) to result in a state-of-the-art modeling system suitable for conducting source-receptor assessment studies, (2) to be sufficiently flexible to integrate current and developing representations of the relevant physical and chemical processes, and (3) to describe the spatial and temporal distributions of pollutants resulting from known source emissions. Progress toward these objectives has been very favorable. A first version of the RADM was completed in January 1985 and since that time has undergone numerous sensitivity studies and preliminary evaluation against existing field and laboratory data. A summary of the preliminary evaluation of the RADM and of sensitivity and application studies is presented here. The evaluation of the RADM submodels are discussed first. Next, 72-h RADM simulations of two OSCAR (Oxidation and Scavenging Characteristics of April Rains field study, conducted in the northeastern United States in April 1981) cases are compared to measured precipitation chemistry data. For one of these cases, a preliminary evaluation of the meterological model is presented. Emissions sensitivity studies and emissions reduction experiments are also presented for one of the OSCAR cases. Finally, databases available for evaluation of the RADM and their limitations are discussed.

RADM Submodel Evaluation

The RADM version I gas-phase chemistry mechanism has been compared with both smog chamber data and more complex chemical mechanisms. In general, these tests show that the RADM mechanism gives a good representation of those aspects of tropospheric chemistry necessary for the modeling of acid deposition. Initial tests were made with data obtained from the Satewide Air Pollution Research Center (SAPRC), and agreement between RADM simulations and experimental values is generally very good for NO_2, NO, and O_3. The agreement between the predicted and experimental values for all the reactive species is excellent. Since reactions with HO radicals is the dominant loss process for reactive organics during photooxidation, the agreement between the simulation and measured concentrations of reactive organic species shows that the RADM mechanism is correctly predicting HO concentrations within the uncertainty imposed by wall sources.

Comparison of the RADM gas-phase chemistry predictions with the University of North Carolina smog chamber data is only in the beginning stages. Procedures used to establish the error bounds of these data, along with comparisons with RADM predictions for a single case, are reported. In general, RADM predictions for O_3, NO, and PAM are in good agreement with the chamber data, considering the uncertainties of the J-values. The simulation also suggests that for definitive tests of the chemical mechanisms for the production of H_2O_2 in the atmosphere, the photolytic rate constant must be accurately known.

The RADM gas-phase chemical mechanism was compared to the explicit mechanism of Leone and Seinfield and the carbon bond mechanism, version CBM-X, for conditions ranging from very clean to highly polluted. Both of these latter mechanisms were modified to include sulfur chemistry. Oxidation rates for SO_2 and NO_x are in reasonable agreement by the three mechanisms, while large differences exist for the total H_2O_2 produced. A sensitivity analysis was performed to determine reasons for the differences in H_2O_2.

The RADM cloud processes and aqueous-phase chemistry module was subjectively evaluated against limited field data and more complex models. Comparisons with OSCAR aircraft observations of cloudwater composition suggest that the RADM submodel is capable of inferring cloudwater pH over the range of initial conditions encountered during the observation period. RADM predictions of aqueous oxidation within clouds are shown to agree reasonably with the difference in the ratio of SO_2 to total sulfur at the base and top of typical cumulus clouds. Scavenging ratios predicted by the RADM are shown to lie between the extremes observed in field observations. In addition to predicting cloud and rainwater composition, the RADM cloud processes model also predicts the rate at which pollutants are vertically transported by sub-grid scale cumulus clouds. RADM parameterization for this process was compared to a high resolution cloud model, and both predicted similar significant depletion of a passive tracer from the boundary layer and "venting" of this material to the cloud layer.

The method used by the RADM to model dry deposition assumes a series of three resistances (aerodynamic, sublayer, and surface) and is based on a highly empirical parameterization, relying heavily on a relatively sparse database of dry deposition measurements. Therefore, it was not possible to evaluate independently the performance of the dry deposition model since all available measurements of dry deposition have been used to tune the current model parameterizations. Data needs for comprehensive dry deposition model evaluation include heat and momentum fluxes in the surface layer, wind speed, isolation, land type (onto which substances are deposited), surface roughness, and a quantification of surface moisture.

Preliminary Evaluation of RADM with OSCAR Database

The overall performance of the meteorological model and RADM in predicting the meteorological processes and wet concentration/deposition during the OSCAR IV period (April 22-24, 1981) was examined. A number of quantitative measures of the accuracy of the mesoscale meteorological model are described. These measures will be used to compare the accuracy of different versions of the mesoscale model and to provide quantitative estimates of the error in the meteorological data supplied to the RADM. Interpretation of the verification scores and methods from the OSCAR IV case are provided.

Correlations between RADM model results and OSCAR measurements of precipitation chemistry variables are presented for two OSCAR cases for both hourly and event totals of concentrations and deposition. Parameters compared were sulfate, nitrate, ammonium and hydrogen ions in rainwater. In all cases, the correlations were much higher for the total event comparison and for concentrations. Correlations were also higher for the OSCAR IV case than OSCAR I.

RADM Sensitivity Studies and Applications

Ultimately, RADM will be used to evaluate source-receptor relationships and the effects of changes in emissions on downwind receptors. This requires an understanding of the basis of the patterns of concentration and deposition forecast by the RADM along with sensitivity of the forecasts to various input parameters and physical parameterizations. Toward this end, wet and dry deposition patterns for the OSCAR I and IV cases were analyzed. Results are also presented for RADM simulations of two "what if" scenarios of 50% and 90% source reduction in the Ohio Valley region.

The patterns and magnitudes of dry deposition of SO_2 over the northeastern United States and southeastern Canada integrated over the three-day episodes were similar for both the OSCAR I and IV cases. In Canada, peaks showed up near Sudbury and Noranda. In the United States, the peaks showed up over south-central Pennsylvania; at the conjunction of Ohio, Pennsylvania, and West Virginia; and in New Jersey. A maximum dry deposition of 1.14 kg/ha after three days occurred over south central Illinois during OSCAR IV. For HNO_3, the accumulated dry deposition for the two three-day episodes were again quite similar, and mass deposition was considerably less than SO_2. A maximum deposition of 0.24 kg/ha occurred from northern New Jersey to southern New Hampshire. The accumulated wet deposition differed more between the two experiments than did dry deposition. This reflects primarily the difference in rainfall patterns for the two episodes. The percentage of total sulfur deposition that was wet was about 50% and 60% fo the OSCAR I and IV cases, respectively. The percentage of nitrogen deposition that was wet was 45% and 60% for OSCAR I and IV, respectively.

Several sensitivity tests were run in which the SO_x emissions were reduced by 50% and 90% in the Ohio Valley (states of Indiana, Ohio, Kentucky, Tennessee, and West Virginia). In response to this regional reduction in emissions, the maximum regional reduction for dry and wet deposition occurred in the reduced emissions area, but only weakly in more distant receptor states. The decrease in dry deposition was greater than the decrease in wet deposition only in the four states with decreased emissions. The decrease in sulfur emissions had very little effect on nitrogen chemistry or nitrogen deposition.

Databases for RADM Evaluation Studies

The evaluation of RADM performance requires the assessment of the databases used for model execution and evaluation. Included in the report are a description and evaluation of the available air quality databases for evaluating regional models, a description of quality control procedures employed in preparing the emissions databases (EPRI and NAPAP) for model applications, and the precipitation database used in verification of the precipitation predictions. Also discussed are the limiations of smog chamber data in evaluating RADM chemistry.

The National Center for Atmospheric Research is located in Boulder, CO 80307.
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The complete report, entitled "Preliminary Evaluation Studies with the Regional Acid Deposition Model (RADM)," (Order No. PB 86-175 692/AS; Cost: $22.95, subject to change) will be available only from:
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