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Project Summary

RELMAP: A Regional Lagrangian Model of Air Pollution User's Guide

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The REgional Lagrangian Model of Air Pollution (RELMAP) is a mass-conserving, Lagrangian model that simulates ambient concentrations and wet and dry depositions of SO_2, $SO_4^=$, and fine and coarse particulate matter over the eastern United States and southeastern Canada (default domain). Discrete puffs of pollutants, which are released periodically over the model's domain, are transported by wind fields and subjected to linear chemical transformation and wet and dry deposition processes. The model, which is generally run for one month, can operate in two different output modes. The first mode produces patterns of ambient concentration and wet and dry deposition over the defined domain, and the second mode produces interregional exchange matrices over user-specified source/receptor regions.

RELMAP was written in FORTRAN IV on the Sperry UNIVAC 1100/82, and consists of 19 preprocessor programs that prepare meteorological and emissions data for use in the main program, which uses 17 subroutines to produce the model simulations. The procedure necessary for running the preprocessors and the model is presented in an example execution, which also allows the user to verify his results.

A statistical evaluation of the model reveals that seasonal and annual simulations of sulfur wet depositions for 1980 generally agree within a factor of two with the observed data. The model, which generally overpredicts wet deposition in spring and summer, produced Pearson correlation coefficients that ranged between 0.208 during autumn and 0.689 in spring.

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

During the mid-1970's, SRI International developed a Lagrangian puff air pollution model called EUropean Regional Model of Air Pollution (EURMAP) for the Federal Environment Office of the Federal Republic of Germany. This regional model simulated monthly SO_2 and $SO_4^=$ concentration and wet and dry deposition patterns, and generated matrices of international exchanges of sulfur for 13 countries of western and central Europe.

By the late 1970's, the U.S. Environmental Protection Agency (EPA) sponsored SRI International to adapt and apply EURMAP to eastern North America. The adapted version of this model, called the Eastern North American Model of Air Pollution (ENAMAP), also calculated monthly SO_2 and $SO_4^=$ concentrations and wet and dry deposition patterns, and generated matrices of international exchanges of sulfur for a user-defined configuration of regions.

During the early 1980's, EPA modified and improved the model to increase its flexibility and scientific credibility. By 1985, simple parameterizations of processes involving fine (diameters $< 2.5\ \mu m$) and coarse ($2.5\ \mu m \leq$ diameter $\leq 10.0\ \mu m$) particulate matter were incorporated into the model in response to impending federal standards for inhalable particulate matter. This latest version of the model, called the REgional Lagrangian Model of Air Pollution (RELMAP), is capable of simulating concentration and wet and dry deposition patterns of SO_2, $SO_4^=$, and fine and coarse particulate matter. It can also generate source-receptor matrices of SO_2, $SO_4^=$, and particulate matter for user-defined regions.

RELMAP consists of 19 preprocessing programs that prepare gridded meteorological and emissions data for use in the main program, which uses 17 subroutines to generate the simulations. RELMAP was developed on a Sperry UNIVAC 1100/82, but can be run on other systems with minor changes. RELMAP represents state-of-the-art modeling for the simulation of the transport, diffusion, transformation, and deposition of these pollutants.

One of the main features of RELMAP is its flexibility. The values of more than fifty parameters, which have been defined with default values, can be redefined by the user simply by changing the values in one subroutine. The optimum values of most of the parameters used in the model have been investigated by numerical experimentation, but not all are known. Therefore, the user has the option of specifying other parameter values. As more knowledge is gained about the parameterizations used by the model, new values can be substituted, thereby making RELMAP a constantly evolving model.

Input data required by RELMAP can be divided into three major categories: (1) meteorological, which include surface and 850 mb winds, precipitation, and monthly maximum mixing heights; (2) emissions, which include point (stack) and area sources of SO_2, $SO_4^=$, and fine and coarse particulate matter; and (3) terrain data, which are defined by land use types. All input data must be converted from their original raw forms into the gridded forms required by the model. This requires spatial interpolation of the data from reporting stations to grid cells with a user-defined (1° x 1° = default) resolution. Temporal interpolation is also required to convert the time increments of the raw data, which vary from 1 h to 12 h, into the user-defined time increment of the model (2 h = default).

Output can be generated in two major formats. The first format generates user-defined (45 x 30 = default) arrays of gridded values of ambient concentrations and wet and dry deposition of SO_2, $SO_4^=$, total sulfur, and fine and coarse particulate matter. The second output format, which considers the same parameters, produces source-receptor exchange tables. With both output formats, depositions are given in kilograms per hectare, and concentrations are given in micrograms per cubic meter. A budget of the total sulfur and particulate matter throughout each model simulation precedes the output arrays. This budget table contains total pollutant input into the model, total wet deposition and total dry deposition of the pollutant, the amount that was transported off the grid, the amount of pollutant that remained in puffs at the completion of each run, and when applicable, the amount of pollutant transformed (e.g., SO_2 into $SO_4^=$).

Theoretical Basis of the Model

RELMAP is a mass-conserving, regional-scale Lagrangian model that simulates ambient concentrations as well as wet and dry depositions of SO_2, $SO_4^=$, and fine and coarse particulate matter. The model performs simulations on a user-defined latitude-longitude grid with a user-defined degree of resolution (approximately 10,000 km^2 with the default 1° x 1° grid) covering the eastern two-thirds of the United States and southeastern Canada. The north-south, east-west boundaries of the model's default domain extend from 25° to 55°N latitude and from 60° to 105°W longitude, respectively.

RELMAP divides the atmospheric boundary layers into three layers, into which seasonal emissions are injected. The first layer is between the surface and 200 m, and the second is between 201 and 700 m. The depth of the third layer depends on the maximum mixing height. Default values vary between 1150 m in winter, to 1300 m in spring and fall and 1450 m during the summer.

In the default mode, discrete puffs of SO_2, $SO_4^=$, and fine and coarse particulate matter are released every 12 h for each of the 1350 grid cells that contain sources. By using vertically integrated and horizontally and temporally interpolated wind fields the model transports each puff in user-specified time increments until the puff is either transported out of the model's domain or until the mass of the pollutant falls below a user-specified minimum value. The pollutants in each of the three layers of a puff are transported in the same direction at the same speed (i.e., the puff remains an indivisible entity).

RELMAP parameterizes both the horizontal and vertical diffusion of the puffs very simply. During the unstable regimes of midday periods, pollutants from both point and area sources become well mixed below the mixing height long before the pollutants are transported a distance comparable to the spatial resolution of the default grid. For this reason, it is assumed that instantaneous, complete mixing within the three layers of the model occurs during the unstable daylight hours. After sunset, when mixing is prohibited by stable conditions, point-source and area-source emissions are injected into separate layers and confined to those layers. All emissions from area sources remain in Layer 1, within 200 m of the surface. Emissions from point sources are allocated into Layer 2, accounting for typical plume rise, which averages several hundred meters. Horizontal diffusion of the puffs occurs at a constant rate, so that the area of each puff increases at a rate of 339 km^2/h, with the mass of the pollutant remaining homogeneous in the horizontal at all times. Linear chemical transformation and wet and dry deposition processes are simulated by RELMAP as each puff is transported across the model's domain. For each time step, the suspended mass and deposition of each puff are apportioned into the appropriate grid cells, based on the percentage of puff over each grid cell.

RELMAP treats fine and coarse particulate matter as independent, nonevolving pollutants; that is, physical and chemical transformations between fine and coarse particles are considered to be negligible. This premise is supported by particle size distributions obtained from monitoring data, which exhibit a bimodal distribution with peaks in the fine and coarse particle ranges and a deep gap oscillating between 1 and 5 μm. RELMAP does, however, consider the transformation of SO_2 into $SO_4^=$. In the atmosphere, this rate varies nonexclusively with solar insolation (and thus time of day, time of year, and latitude) and moisture content. RELMAP simulates the transformation of SO_2 to $SO_4^=$ through the use of a heterogeneous component and a homogeneous component. The heterogeneous component accounts for the more rapid transformation processes that occur in saturated environments, while the homogeneous component simulates transformation that occurs under dry conditions. Both components vary seasonally.

Dry deposition of SO_2, $SO_4^=$, and fin and coarse particulate matter is a highl variable, complex process that i parameterized by RELMAP as a functio of predominant land use, season, an stability. Twelve land use categories, de fined by surface characteristics and vegetation type have been gridded to RELMAP's 1° x 1° grid. Dry deposition velocities, which represent the downward surface flux divided by the local concentration, were calculated for each land use type, for six different stability classes and for each season for SO_2, $SO_4^=$, and fine and coarse particulate matter. The dry deposition velocities for SO_2 range between 0.05 and 1.15 cm/s, and $SO_4^=$ and fine particulate matter, velocities range between 0.05 and 0.50 cm/s. During the nighttime hours, the dry deposition velocities for SO_2, $SO_4^=$, and fine particulate matter are reduced to 0.07 cm/s, in order to compensate for the very high nocturnal resistance, when plant absorption is minimal.

Because coarse particulate matter consists of a wide range of particle diameters, two sets of dry deposition velocities are used by the model. The first set applies to particulate matter with diameters of 5 μm, and the second set applies to particles with diameters of 10 μm. The dry deposition velocities for particles with a 5-μm diameter range between 0.4 and 5.0 cm/s, and between 1.0 and 6.0 cm/s for 10- μm diameter particles. Unlike SO_2, $SO_4^=$, and fine particulate matter, the dry deposition velocities of coarse particulate matter are much less dependent on the time of day and the season; therefore, diurnal and seasonal variation are considered negligible.

The complex process of wet deposition of SO_2, $SO_4^=$, and fine and coarse particulate matter is thought to be a function of cloud chemistry and cloud type, pollutant concentration, and precipitation type and rate. RELMAP, however, parameterizes wet deposition quite simply, treating it as a function of season and precipitation rate only. The wet deposition rates are expressed as percentages per time step, which depend solely upon precipitation rate and cloud type. Three cloud types were considered including Bergeron or cold-type clouds, warm or maritime-type clouds, and convective-type clouds. RELMAP assumes that all winter precipitation results from the Bergeron process, that spring and autumn precipitation result from warm cloud formation, and that summer precipitation is produced by convective-type clouds.

Model Performance Evaluation

In general, a rigorous evaluation of any model requires a long-term reliable data set consisting of measurements of all parameters simulated by the model across a network of representative sites similar to the spatial and temporal resolution of the model. Unfortunately, such a complete data set is not available to rigorously evaluate all aspects of RELMAP. However, a spatially and temporally consistent sulfur wet deposition data base is available to evaluate the model. Such a data set was acquired from the Acid Deposition System (ADS), operated for EPA by Pacific Northwest Laboratory.

Monthly simulations of concentrations and wet and dry depositions of SO_2, $SO_4^=$, and total sulfur were made for all of 1980. Emissions data used in simulations were from the 1980 National Acid Precipitation Assessment Program (NAPAP) Task Group B emissions inventory (Version 2.0) and from the Environment Canada emissions inventory used in Phase III of the U.S./Canadian Memorandum of Intent on Transboundary Air Pollution. Seasonal and annual predictions of sulfur wet deposition (expressed in kilograms of $SO_4^=$ per hectare) were compared to the amount of seasonal and annual sulfur wet deposition recorded by the ADS system. The number of observations for the seasonal evaluations ranged from 36 in the winter to 43 during the spring. The annual evaluation consisted of 34 observations.

Comparison of the means and standard deviations of the predicted and observed values, with their corresponding residuals, provides an indication of the model's overall performance. RELMAP slightly overpredicted total sulfur wet deposition during the winter (0.01 kg $SO_4^=$/ha, or 0.22%). It overpredicted wet deposition during the spring (2.02 kg $SO_4^=$/ha, or 25.73%) and summer (3.43 kg $SO_4^=$/ha, or 37.12%). It underpredicted for autumn (0.37 kg $SO_4^=$/ha, or 9.23%). In the annual simulation, the model over-predicted total sulfur wet deposition (5.41 kg $SO_4^=$/ha, or 20.66%). The percentages of over/underprediction were calculated by dividing the residuals by the mean of the total observed sulfur wet deposition by season. Examination of the standardized residuals indicates that there is a consistent tendency within each season for the model to overpredict total sulfur wet deposition in the major source regions (i.e., Ohio River Valley) and to underpredict wet deposition in the nonindustrial areas.

The pronounced overprediction that occurs during the spring and summer can in part be attributed to two major factors: (1) the model does not account for sub-grid-scale precipitation variability, and (2) the model does not account for the vertical transport of pollutants from the mixed layer into the free troposphere by cumulus cloud venting. RELMAP assumes that precipitation occurs everywhere within a grid cell whenever precipitation occurs at any site within that cell. Therefore, the frequency of simulated precipitation events in any grid cell is higher than the actual frequency at one site in that cell, especially during the months of convective-type precipitation (spring and summer). Consequently, wet deposition will occur more frequently in the simulations.

In support of the second factor attributed to model overprediction, it is estimated that clouds vent 20% of the subcloud layer air into the troposphere during winter and 50% during summer. Failure to account for such vertical transport could result in excessive sulfur wet deposition occurring near the source regions, especially during the convective seasons (spring and summer), which is consistent with the analysis.

Seasonal scatter diagrams, which exhibit the correlation or dependency of the predicted values on the observed values, reveal that the model produced higher correlations during the spring (0.689) and summer (0.562) than it did during autumn (0.208) and winter (0.479). The annual simulation produced a Pearson's correlation coefficient of 0.614, indicating that 37.7% of the variance exhibited by the observed data could be accounted for by the simulation.

Computer Aspects

The RELMAP model consists of two major components, the preprocessors and the model itself. The software for RELMAP is written in ASCII FORTRAN and was developed and tested on the Sperry UNIVAC 1100/82 at the National Computer Center at the U.S. Environmental Protection Agency in Research Triangle Park, North Carolina. Three UNIVAC-specific routines are used in the software: ADATE, SORT, and ATAPE. If the user has a different computer system, comparable routines must be used.

In its most complex form, the model requires five types of preprocessed input data (upper-air data, surface data, precipitation data, emissions data, and dry deposition velocity data). The preprocessors should be run in sequence, because the output file format of one program is the input file format for the next sequential program. Therefore, once the user has formatted the first file in the sequence, he does not have to format the remainder of the files, because their formats are identical.

The RELMAP model itself consists of one primary program (MAIN) and 17 subroutines, which are called by MAIN. Besides calling the subroutines, this program performs a number of other functions such as determining when puffs should be generated, tracking the number and location of puffs, implementing the chosen output mode, and defining vertical profiles of the pollutants. MAIN also contains all the COMMON blocks used by the model to pass information.

An example execution of the RELMAP model and its preprocessors, which uses the Executive Control Language (ECL) of the Sperry UNIVAC system, is provided. In this example execution, the preprocessors and both output versions of the model are run for the month of January 1980 for a 12° x 13° window located within the model's default domain. This window, which extends from 30° to 43°N and from 80° to 92°W, contains a total of 156 grid cells.

An annotated precis of the tape that accompanies the user's guide is presented in the full report, which contains a brief description of the 14 files on the tape. The first four files are program files that contain the program elements for the model and the preprocessors; the ten remaining files contain the data necessary to perform the example execution.

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The complete report, entitled "RELMAP: A Regional Lagrangian Model of Air Pollution User's Guide," (Order No. PB 86-171 394/AS; Cost: $16.95, subject to change) will be available only from:
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