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Project Summary

User's Guide for the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model

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The Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) model simulates long-range, long-term transport and deposition of air pollutants, primarily oxides of sulfur and nitrogen. The ASTRAP model is designed to combine ease of exercise with an appropriate detail of physical processes for assessment applications related to acid deposition. The theoretical basis and computational structure of the ASTRAP model are described. Major simplifications and assumptions incorporated in the model are discussed.

The data requirements for ASTRAP simulations are monthly to seasonal time series of transport wind and precipitation analyses and an emissions inventory. ASTRAP consists of three programs: HORZ, VERT and CONCDEP. The source code is in standard FORTRAN, while the JCL is appropriate for an IBM 3033 mainframe computer. Horizontal dispersion and wet deposition statistics are calculated in HORZ. The process of turbulent vertical diffusion within the mixed layer, leakage to the free atmosphere, chemical transformation and dry deposition are calculated in VERT. The CONCDEP program combines the statistics produced by HORZ and VERT with an emissions inventory to calculate primary and secondary pollutant surface concentrations along with wet and dry depositions.

This Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle P-rk, 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 Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) model described here has been developed to simulate the long-term (monthly to yearly), regional-scale (resolution about 100 km) deposition of oxides of sulfur and nitrogen, the major contributors to acid deposition. The ASTRAP techniques can be extended to other pollutants, provided that linear parameterizations of chemical transformation and removal processes are suitable. They also can be extended to other spatial scales, if appropriate meteorological data are available. Unmodified extension of the modeling techniques used in ASTRAP to shorter, episodic temporal scales is not recommended because of certain statistical features of the model.

The ASTRAP model consists of three submodels and various preprocessors and postprocessors. Use of particular preprocessors and postprocessors depends on application and data availability. The submodels are the vertical diffusion program (VERT), the horizontal dispersion program (HORZ), and the concentration and deposition program (CONCDEP). The processes of vertical diffusion, chemical transformation, and dry deposition are simulated in VERT through parameterizations that are independent of horizontal location or particular meteorological conditions. In HORZ, the processes of horizontal advection, horizontal diffusion, and wet deposition are simulated through the use of time series of wind and precipitation analyses. The CONCDEP program combines the statistics produced by the first two programs with emission inventories to produce fields of average atmospheric concentration and cumulative deposition.

The ASTRAP model can be applied in emission policy assessments, for which the model can be exercised to predict how deposition fields would change in response to changes in the pollutant emission field. Assuming linearity between emissions and deposition, the model can be used to estimate concentration and deposition at specific receptor locations, and it can estimate the individual contribution from different sources or source regions. The following major simplifications and assumptions have been incorporated into the ASTRAP model:

1. Long-term horizontal and vertical dispersion can be simulated independently.
2. Long-term horizontal diffusion can be approximated by the spread of plume centerlines; small-scale diffusion about individual plumes is ignored.
3. Chemical transformation can be parameterized as a linear, first-order process.
4. Wet removal is a function of the half-power of the precipitation.
5. Transport is two-dimensional.
6. The dry deposition parameterization is horizontally uniform.

The data requirements for ASTRAP simulations are monthly to seasonal time series of transport wind and precipitation analyses and an emissions source inventory. Initial preparation of wind and precipitation fields for ASTRAP simulations has been performed at the University of Michigan by Perry Samson. His initial wind fields, produced every 12 h are for 500-m layers up to 3000-m MSL for a 17 x 19 horizontal grid of National Meteorological Center (NMC) spacing. Speed is given in meters per second. Linear temporal interpolation has created fields at 6-h intervals, and the wind analyses have been combined into three-month-long files (December-February, March-May, June-August, and September-November). The wind components have been internally converted to components along the NMC axes in the HORZ subprogram.

The precipitation analyses produced at the University of Michigan are on a 50 x 45 grid with 1/3 NMC spacing. The original analyses are hourly; there is a special code for missing data. Precipitation amount is given in millimeters. The hourly fields have been added to produce six hourly fields; the missing data were filled by interpolation and extrapolation. The precipitation data are arranged on monthly files.

An SO_2 inventory has been created in which the seasonal emissions in kilotonnes are given by effective stack layer and NMC position of the lower left corner of the grid cell. No separate $SO_4^=$ emissions inventory is used, so primary sulfate emission factors are applied in CONCDEP. The primary sulfate emission factor for sources in the lowest layer (0-100 m) is assumed to be 0.05 (i.e., one unit of SO_2 equivalent emission is treated as 0.95 units of SO_2 and 1.5 (0.05) = 0.075 units of primary sulfate; the 1.5 factor arises because the ratio of the molecular weight of sulfate to that of SO_2 is 96/64). The primary sulfate emission factor for point sources is assumed to be 0.03 in Florida and the northeast and 0.015 elsewhere. The emission grid has the same spacing as the precipitation grid, but it is irregular because the inventory is arranged by state and province. The emission information has been derived from a preliminary version of the National Acid Precipitation Assessment Program (NAPAP) inventory for 1980. Wind, precipitation, and emission data are all written in binary format for efficiency.

Technical Description

Horizontal dispersion statistics are calculated in HORZ for a virtual source grid covering the contiguous United States and Canada for a particular meteorological period and are subsequently interpolated when concentrations and depositions are calculated. For a one-to-three-month sequence of meteorological analyses, simulated tracers of unit mass are released from the sources at 6-h intervals. Calculations in HORZ are independent of the height of release. The tracers are tracked for 28 time steps (seven days) or until they leave the wind grid. At each successive tracer position, the precipitation field is checked to see whether there should be wet removal.

The statistics calculated in HORZ are ensemble statistics; each ensemble represents all trajectory positions of a particular plume age for each source for the length of the meteorological analysis. The statistics generated for a puff describing the density of the ensemble of equal age trajectory end points are the coordinates μx and μy of the mean position, the standard deviations σ_x and σ_y, the correlation term ρ_{xy}, and n, the number of equivalent tracer masses contributing to the ensemble statistic. The statistics are collected for a puff associated with airborne or dry tracers and for another puff associated with wet deposition tracers.

The wet deposition is parameterized as a function of the half-power of the precipitation. It contains certain constraints such that any precipitation amount larger than 1 cm/6h has the same effect as that of 1 cm/6h, while precipitation amounts less than a minimum threshold value of 1 mm/6h have no removal effect at all.

As previously mentioned, there are separate sets of statistics for wet and dry tracer ensembles. The same trajectory end points are used in calculation of each corresponding pair of wet and dry ensembles, but the weights are different (most of the wet ensembles have zero weight) and, thus, the wet and dry ensemble puffs differ. The puffs for dry deposition and surface concentration tend to be more regular in the trend of their overlapping positions than do the wet deposition puffs. This is because wet deposition is a highly irregular process and thus exhibits more statistical variation for a single season.

The process of turbulent vertical diffusion in the mixed layer, leakage to the free atmosphere, chemical transformation, and dry deposition are calculated in the VERT program. The diurnal variation of the planetary boundary layer is parameterized in VERT through a seasonally and diurnally varying stability profile (vertical eddy diffusivity specified for each layer of the model).

The variations in dry deposition amounts associated with typical diurnal and seasonal patterns of both atmospheric stability and surface resistances are parameterized through average diurnal values of dry deposition velocities for each season. A diurnal variation in the linear first-order transformation rate of the primary pollutant (SO_2 or NO/NO_2) to a secondary pollutant ($SO_4^=$ or NO_3) directly or indirectly due to photochemical activity patterns is also compensated for in VERT. The seasonal patterns are intended to include all chemical transformation pathways except those associated with precipitating clouds. The rates of SO_2 transformation, for example, are greater than those normally found in clear-air experiments, because the rates include the effects of chemical processing in nonprecipitating clouds.

Leakage from the mixed layer into the free atmosphere is now parameterized in ASTRAP, but the rates have been set at relatively low values until more is learned about the long-term regional significance of the layer.

The calculated and stored normalized statistics from the VERT program for a seasonal simulation include the one-dimensional surface concentration, the pollutant mass remaining aloft, and the pollutant mass deposited by dry processes during the time increment. Separate sets of statistics are maintained for SO_2, primary and secondary $SO_4^=$, as well as NO/NO_2, primary and secondary NO_3. The eddy diffusivity, chemical transformation, and dry deposition parameterizations for a particular season are applied everywhere, regardless of latitude or surface vegetation. This is an obvious limitation of the ASTRAP algorithms, which include some oversimplifications to achieve computational simplicity and efficiency.

The CONCDEP program combines the statistics produced by HORZ and VERT programs with an emissions inventory to calculate primary and secondary pollutant surface atmospheric concentrations and wet and dry depositions. The concentration and deposition fields are calculated by overlaying puffs and adding their densities over the receptor grid. For this, the puffs must be weighted by both the emissions rate per 6 h for the source and the number of normalized tracer masses contributing to the puff.

Emissions from a hypothetical source in Oklahoma were combined with summer vertical dispersion statistics and with trajectory statistics for June through August, 1980, to perform a seasonal simulation in a test of the model. Arrays of the concentration and deposition fields and a table of total deposition for each receptor (state or province) were generated.

Computer Aspects

As currently structured, ASTRAP consists of three programs: HORZ, VERT, and CONCDEP. The job control language is appropriate for the IBM 3033 mainframe computer at the Argonne National Laboratory; it would require some modification for use on other systems. While programming is in standard FORTRAN, input and output algorithms may require coding modification for other systems. On an IBM 3033, VERT requires 210k (bytes) storage, 5-10 min of CPU time, and one output file for a seasonal simulation. HORZ requires 500k storage, 10 min CPU time, two input tape drives, and an output file for a seasonal simulation. CONCDEP requires 500k storage, 10-15 min CPU time, an emission input file, the output files from the other two subprograms, a file used to identify each receptor cell as a state or province, and an output file for a seasonal simulation. The output file from CONCDEP is normally stored on disk, where postprocessors can later be used to display the results graphically.

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The complete report, entitled "User's Guide for the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model," (Order No. PB 85-236 784/AS; Cost: $11.50, subject to change) will be available only from:
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