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Project Summary

SAI Airshed Model Operations Manuals

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The SAI Airshed Model Operations Manuals present a general view of the Systems Applications, Inc. (SAI) Airshed Model as well as detailed operating instructions for the user. The User's Manual includes discussions of all the files needed to run the model, the data preparation programs that produce each file, the input formats and data preparation methods, samples of input and output, and information flow diagrams that illustrate the job stream control on any computer.

The Systems Manual, the companion to the User's Manual, describes the system from a programmer's point of view. Included are descriptions of all subroutines and how they fit together, run-time core allocation techniques, internal methods of segment handling by using secondary storage, and detailed structure definitions of all files in the system. The Systems Manual also discusses procedures for implementing the programs on different computers, and the addition, removal, or replacement of computing algorithms and data preparation methods.

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

The Systems Applications, Inc. (SAI) Airshed Model was designed to calculate the concentrations of both reactive and inert air pollutants through simulation of the numerous physical and chemical processes that take place in the atmosphere. Much of the current interest in the model arises from the need to calculate ozone concentrations as a part of various environmental assessment studies (such as State Implementation Plans and New Source Reviews). The Airshed Model provides a means for analyzing a variety of urban-scale air quality problems.

Interactions among organic compounds (including pure and oxygenated hydrocarbons and hydrocarbon derivatives) and nitrogen oxides (NO_x) are usually responsible for the relatively high ozone concentrations observed in and downwind of urban areas. Among the main factors affecting photochemical air quality in urban areas are:

- The spatial and temporal distribution of emissions of NO_x and organic species.
- The composition of the emitted organic species.
- The spatial and temporal variations of the wind field.
- The stability of the atmosphere and the associated dynamics of the mixing layer.
- The chemical reactions involving organic species and NO_x.
- The diurnal variations in ultraviolet radiation.
- The loss of ozone and its precursors by surface uptake processes.
- The ambient background concentrations of ozone, organic species, and NO_x immediately upwind of the urban area and within an elevated inversion layer.

Thus, development of an accurate ozone prediction relationship requires investigation of the relevant physical and chemical atmospheric phenomena that influence the magnitude and distribution of both ozone and its precursors.

To limit ozone concentrations, one must control all or part of the ozone formation process. Practically, man has the most influence on anthropogenic emissions. If ozone concentrations were proportional to emissions of organic compounds or NO_x, it would be simple to calculate the reduction in anthropogenic emissions necessary to achieve a desired reduction in ozone concentrations. However, the relationship between ozone air quality and emissions of NO_x or organic species is complicated and nonlinear. Furthermore, the relationship changes with location and even with time at a given location because of variations in emissions, meteorology, and other factors.

To make available an appropriate quantitative treatment of this relationship, the U.S. Environmental Protection Agency (EPA) has, through a multiyear research effort, supported the development of the SAI Airshed Model.

The Airshed Model can simulate the dynamic behavior of up to 20 pollutants. When photochemical simulations are carried out, 11 species must be included: nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), single-bonded carbon atoms (PAR), double-bonded carbon atoms except ethylene (OLE), aromatic-bonded carbon atoms (ARO), carbonyl-bonded carbon atoms, ethylene, benzaldehyde (BZA), peroxyacetyl nitrate (PAN), and carbon monoxide (CO). In addition, the model can provide predictions of SO_2 and selected aerosol parameters.

Simulations are performed on a three-dimensional grid selected by the user to cover the region of interest. The base of an elevated inversion layer is often selected as the top of the grid, but the model includes provisions to facilitate treatment of the inversion layer itself. The model's computer codes can handle any number of cells in the horizontal and vertical directions, although practical considerations of computer storage and time requirements limit the extent of the model domain.

Treatment of Atmospheric Chemistry

Ozone is not emitted from sources; rather, it is formed by chemical reactions in the atmosphere. Consequently, to calculate ozone concentrations, a physicochemical model must contain a kinetic mechanism; that is, a group of chemical reactions and rate constants intended to represent the ozone formation process. Because of computing time limitations, it is not possible to include each chemical species of interest; thus, most of these kinetic mechanisms treat organic compounds in groups, which are often based on reactive functional components they contain.

Because of the association of reactions and reactivities with carbon bonds, the range of reactions and rate constants to be treated in a kinetic mechanism can be narrowed considerably when each carbon atom is treated according to its bond type. This concept is the basis for the Carbon-Bond II Mechanism, a 65-reaction mechanism developed at SAI and employed in the SAI Airshed Model. In this mechanism, the carbon atoms of each organic compound are assigned to one of the following groups: PAR, OLE, ethylene, ARO, carbonyl-bonded carbon atoms, and BZA. The user can optionally include four reactions in the mechanism describing SO_2 oxidation and reaction expressions accounting for the formation of sulfate, organic, and nitrate aerosol products. Simulations of smog chamber experiments indicate that the Carbon-Bond II Mechanism performs significantly better than those previously employed in the Airshed Model.

Treatment of Advective Pollutant Transport

Pollutants are transported primarily by advection, that is, by the mean or bulk motion of the wind. A major difficulty in treating advection is wind shear, the variation of the wind with altitude. The wind speed near the ground typically increases with height, but the wind several hundred meters aloft may be faster or slower—and frequently from a different direction. The Airshed Model has the capability to treat wind shear phenomena. One or more objective techniques are used to prepare appropriate three-dimensional wind inputs to the model.

Treatment of Turbulent Diffusion

Pollutants are transported and dispersed largely by the action of the wind rather than by molecular diffusion. The above discussion of advection does not represent pollutant transport completely because it ignores the influence of small-scale features of the wind, eddies. Describing these microscale features of the wind deterministically is difficult because available data are insufficient to characterize winds on such a fine scale. Consequently, it is necessary to parameterize the microscale turbulent diffusion processes. In the SAI Airshed Model, and in most other grid models as well, transport of a pollutant by turbulent diffusion is assumed to be proportional to the rate of change of concentration with position (i.e., concentration gradient). The proportionality factor is termed the eddy diffusivity coefficient. These coefficients are sometimes treated as constants, but they can more accurately be treated as functions of atmospheric stability, surface roughness, and height above the ground.

Because of the empirical nature of the eddy diffusivity concept, it has up to this time been difficult to obtain precise measured or theoretical estimates for the diffusivity coefficients. The approach taken in the Airshed Model uses control theory techniques in conjunction with the results of a sophisticated planetary boundary layer model to generate "optimal" diffusivity values.

Treatment of Surface Removal Processes

Many types of pollutants, including NO_2, O_3, and SO_2 in particular, can be removed from the atmosphere by chemical reaction, adsorption, or absorption at various surfaces found in urban areas. A methodology for calculating the removal of gaseous pollutants by surface sinks has been incorporated in the model. Surface removal is assumed to take place in two steps: transport to the surface followed by uptake by the surface. Parameterization of this two-step process is accomplished by defining a resistance to mass transport and a resistance to surface removal. The transport resistance is estimated from theoretical considerations of turbulent transfer in the atmospheric boundary layer, and the surface resistance is obtained from experimental data on the uptake of pollutants by various types of surfaces.

Other Technical Features

The numerical procedure used to solve the conservation-of-mass equations for each pollutant is an important component of a grid model. To minimize the propagation of numerical errors, techniques for treating horizontal (advective) pollutant transport (an element of the model particularly difficult to handle numerically) were examined. The results of these

studies indicated that, of the techniques examined, the SHASTA integration scheme provided the best balance between accuracy of prediction and computational speed.

The SAI Airshed Model contains features designed to reduce cost by minimizing labor and computing expenses. For example, computerized data preparation programs are available for automating the conversion of various types of data into the proper input format. These features have no effect on the model's treatment of atmospheric processes, but they do aid the user in preparing the inputs required by the Airshed Model.

The model output consists of the predicted pollutant concentrations for every grid cell. These predictions are generally averaged over a period of one hour and are saved on a computer file for subsequent display and analysis. Gridded census data can be used in conjunction with the model predictions to estimate the dosages and exposures that are experienced by the human population within the modeling region. Other displays and analyses can be prepared depending on the needs of the user.

Overview of the System

The SAI Airshed Model System contains at its core the Airshed Simulation Program, the input data that consist of 10 to 14 files depending on the program options chosen. Each file is created by a separate data preparation program. There are 17 programs in the entire Airshed Model System. The output from the Airshed Simulation Program consists of three data results files and an execution trace report. The output data files can be further processed by the display and analysis programs and can also be used for restarting the simulation.

The Airshed Model System can be described according to the five major tasks or functions that the user and the programs must perform:

- M.E.B. (meteorology, emissions, and initial and boundary conditions) file preparation.
- M.E.B. file segmentation.
- Control data preparation.
- Airshed simulation.
- Display and analysis.

This classification of programs and tasks is used as the organizational basis for both the User's Manual and the Systems Manual.

Of the 14 files input to the Airshed Simulation Program, two are classified as "control files." The remaining 12 files are the M.E.B. files. The Airshed Simulation Program requires appropriate meteorological, emissions, and initial conditions data for each cell of the region's rectangular grid. In addition, the concentration of each pollutant must be specified at each point on the boundary where the wind is flowing into the region. These data enter the program through the M.E.B. files.

For each file, there is a data preparation program that takes either observations or estimates at specific locations in the region, creates a fully gridded data field, and writes the data to the file in the appropriate format. The 12 M.E.B. data preparation programs are designed to be used together as a unified, user-oriented package. The input formats to all the programs are standardized and reasonably self-documenting. The interpolation methods are intended to accommodate input data of any complexity, from variables for which little or no data are available to those for which there are many observations and well-known interactions. Also, the units of measure are standardized, a flexible unit conversion scheme is built into the programs.

The M.E.B. data preparation function consists of the following tasks for the user:

- Determination of the appropriate files for a given simulation.
- Detailed examination of the data requirements and optional methods for each file.
- Translation of available data into a form acceptable to the model.
- Selection of the proper interpolation methods.
- Establishment of the size and location of the region.
- Establishment of the vertical distribution of cells within the region.
- Exercise of the data preparation programs, examination of the results, and modifications of the inputs or algorithms until a reasonable set of data is produced.

The preparation of the M.E.B. data files is certainly the most difficult and time-consuming task associated with use of the SAI Airshed Model System. It is also the most important task, and careful, intelligent creation of the input is required to yield the best simulation results.

The SAI Airshed Model System has been designed to enable simulation on a rectangular grid of any size and shape; that is, the dimensions of the region are not fixed within the programs but are specified at run time. If a specified region does not fit within the core limitations of the host computer, that region can be divided into any number of contiguous subrectangles called "segments"; in this case, the size of each segment, rather than the size of the entire region, is limited by the amount of core available. The Airshed Simulation Program processes each segment in turn, and information at the interfaces between segments is maintained.

The Airshed Simulation Program requires two control files: the Chemistry Parameters file (CHEMPARAM), and the Simulation Controls file (SIMCONTROL), each created by its own data preparation program.

For the CHEMPARAM file, all chemical species to be simulated are named and their properties are specified. This list of species, rather than the lists that appear on any of the other data files, determines which species will be simulated. If there are any reactive species, the reaction rate constants and their other properties (such as the activation energy and reference temperature) are also specified. The user's tasks in making the CHEMPARAM file are:

- Preparation of a card deck describing the species and the chemical mechanism to be used.
- Running the program that creates the CHEMPARAM file.

The SIMCONTROL file includes values for the simulation options, time span, integration controls, and output options, which are the data likely to be changed most frequently. The user's tasks in generating this file are:

- Proper specification of all input files to be used.
- Arranging to save the output files that the program creates.

The final function of the SAI Airshed Model system is the display and analysis of the simulation results. This function has been removed from the Airshed Simulation Program because often, no matter which output options are selected for a simulation run, different options are needed at a later time. By writing the concentration predictions of all species in all

dimensions to output files, one can select any available output mode at any later time.

The current display program capabilities include printout of either instantaneous or average concentation grid maps for selected species at selected vertical levels at selected times. Instantaneous or average vertical concentration profiles can also be printed at user-specified stations. The user's tasks in running the display program are:

- Proper specification of all input files required (including the desired output file from the Airshed Simulation Program).
- Preparation of an input deck containing parameters for the selection of times, species, and vertical levels to be printed, and station locations where vertical concentration profiles will be printed.

In addition, the design of the display program provides for the inclusion of additional analysis capabilities without extensive modification of the program. Specifically, the structure permits the comparison of two concentration data files. The two data files could be the output from two simulation runs (comparing different control strategies, for example) or one file could be simulation predictions and the other could be a gridded representation of station observation data.

All SAI Airshed Model programs are written in FORTRAN IV (using FORTRAN-66 compiler features) and were originally implemented on the Lawrence Berkeley Laboratory CDC 7600 computer system. The programs were subsequently modified to run on the U.S. Environmental Protection Agency's UNIVAC 1100 computer. The following are some features of the code for this system:

- There are no multiple entry points or returns.
- No arrays are greater than three-dimensional.
- There are no complex or double-precision variables.
- There is no rereading of input data cards.
- All alphanumeric variables are represented by vectors containing one character per word, left justified.
- Output format statements use Ho rith counts rather than special delin ers for alphanumeric text fields.
- Routines accessing secondary stora files or large core memory are isola modules that can be easily change
- All main programs begin with co ments naming all files that the p gram uses and, if necessary, providi equivalences between local file nam and FORTRAN unit numbers.

A magnetic computer tape contain the model code and sample input a output data will be available from t National Technical Information Serv (NTIS), Springfield, VA.

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The complete report consists of two volumes, entitled "SAI Airshed Model Operations Manuals:"

"Volume I. User's Manual," (Order No. PB 85-191 567/AS; Cost: $35.50)

"Volume II. Systems Manual," (Order No. PB 85-191 575/AS; Cost: $20.50)

The above reports will ba available only from: (costs subject to change)

National Technical Information Service
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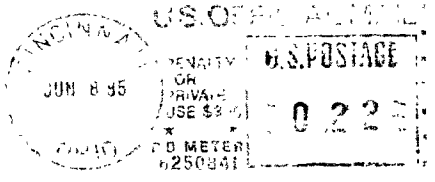

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