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Project Summary

User's Guide to the MESOPUFF II Model and Related Processor Programs

J. S. Scire, F. W. Lurmann, A. Bass, and S. R. Hanna

A user's guide has been assembled to describe the design and operation of the MESOPUFF II regional-scale air quality model. MESOPUFF II is a Lagrangian variable-trajectory puff-superposition model that has been designed to treat transport, transformation, diffusion, and removal processes of pollutants emitted from multiple point and/or area sources at transport distances beyond the range of conventional straight-line Gaussian models (i.e., beyond ~ 10-50 km).

The major features of this model and enhancements over its predecessor, MESOscale Puff (MESOPUFF), include the use of hourly surface meteorological data, twice-daily rawinsonde data, and hourly precipitation data; separate wind fields to represent flows within and above the boundary layer; parameterization of vertical dispersion in terms of micrometeorological turbulence variables; transformation of sulfur dioxide (SO_2) to sulfate ($SO_4^{=}$) and nitrogen oxides (NO_x) to nitrate (NO_3^-); a resistance model for dry deposition; time- and space-varying wet removal; and a computationally efficient puff sampling function. The scientific and operational bases of the methods used in the model are briefly discussed. Complete user instructions and test-case input/output are provided for each program.

This Project Summary was developed by EPA's Environmental 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 regional and long-range transport and transformation of sulfur oxides and nitrogen oxides emitted from major point sources have been of considerable concern. There is a need for easily usable, cost-efficient air-quality models that can realistically treat the various physical processes important on these scales. The MESOscale Puff (MESOPUFF) model has been extensively modified to revise and more realistically treat the transort, vertical dispersion, chemical transformation, and dry and wet removal processes. The new model, designated MESOPUFF II, is one element of an integrated modeling package that includes components for preprocessing of meteorological data (READ56, MESOPAC II) and for postprocessing of predicted concentrations (MESOFILE II).

Major Model Features

MESOPUFF II uses a puff-superposition approach to represent continuous plumes. The pollutant material in each puff is transported independently of that in other puffs and is also subjected to dispersion, chemical transformation, and removal processes. Some of the general features of the MESOPUFF II modeling system are as follows:

(1) Hourly surface meteorological data, twice-daily rawinsonde data, and hourly precipitation data are read from magnetic tapes.

(2) Wind fields to represent the mean flow in the boundary layer and above the boundary layer are constructed, although several options are given.

(3) Boundary-layer structure is treated in terms of micrometeorological parameters that include the surface friction velocity, mixing height, convective velocity scale, and Monin-Obhukov length.

(4) Space- and time-varying chemical transformation can be performed simultaneously for up to five pollutant species, including sulfur dioxide (SO_2), sulfate ($SO_4^=$), nitrogen oxides ($NO_x=NO+NO_2$), nitric acid (HNO_3), and nitrate (NO_3^-).

(5) Dry deposition is prescribed by a resistance model in the surface-depletion mode, and the source-depletion method is optional.

(6) Space- and time-varying wet removal is parameterized according to precipitation rate and scavenging coefficients.

The meteorological data inputs required by the preprocessors consist of the routine twice-daily upper air soundings, hourly surface meteorological observations, and hourly precipitation measurements reported by the National Weather Service. The preprocessor programs have been designed to read the standard-formatted meteorological data tapes available from the National Climatic Center in Asheville, NC.

Wind fields for MESOPUFF II are constructed from the hourly surface wind observations, as well as from the twice-daily rawinsonde wind profile data. The surface station network data allow better temporal and spatial resolution than do the upper air sounding data, which involve much larger distances and less frequent measurements. The wind fields are constructed at two user-specified levels--a lower level representing the mean boundary-layer flow and an upper level representing flow above the boundary layer.

Boundary-layer structure is parameterized in terms of micrometeorological variables computed from the surface station data and information about surface characteristics (land use, or roughness lengths) provided by the user for each grid point. The surface friction velocity, u*, the convective velocity scale, w*, the Monin-Obukhov length, L, and the boundary-layer height z_i, are computed.

Chemical transformation rate expressions were developed from the results of photochemical model simulations over a wide range of environmental conditions. The rate expressions include gas-phase NO_x oxidation, gas- and aqueous-phase components of SO_2 oxidation, and the chemical equilibrium of the nitric acid, ammonia, and ammonia nitrate system. The parameterized transformation rates depend on solar radiation, background ozone concentration, and atmospheric stability. The SO_2 oxidation rate is empirically increased at high relative humidity to account for aqueous-phase reactions. In the case of NO_x, the transformation rate also depends on the NO_x concentration.

The spatial and temporal variations of dry deposition are treated by a resistance model. The pollutant flux is proportional to the inverse of a sum of resistances to pollutant transfer through the atmosphere to the surface. The resistances depend on the characteristics of the pollutant and the underlying surface and atmospheric conditions. MESOPUFF II contains options for the commonly used source-depletion method or for more realistic surface depletion, where pollutants are removed only from a surface layer in the three-layer model.

Precipitation scavenging can be the dominant pollutant removal mechanism during precipitation periods. MESOPUFF II contains a scavenging-ratio formulation for wet removal. The scavenging ratio depends on the type and rate of precipitation (derived from hourly precipitation measurements, if available) and the characteristics of the particular pollutant.

In addition, improvements were made in the method of summing the contributions of individual puffs to the total concentration at a receptor location. The model uses an integrated form of the puff-sampling function that eliminates the problem of insufficient puff overlap commonly encountered with puff-superposition models. This development allows continuous plumes to be more accurately simulated with fewer puffs, thereby saving computational time and reducing computer storage requirements.

MESOPUFF II Modeling System

The MESOPUFF II modeling package is schematically illustrated in Figure 1. The two meteorological preprocessor routines are READ56 and MESOPAC II. READ56 processes the rawinsonde data, and MESOPAC II reads the output file created by READ56 and the standard-formatted hourly surface meteorological data and precipitation data. A single output file is produced that includes all the time- and space-interpolated fields of meteorological variables required by MESOPUFF II. MESOFILE II is a postprocessing program that performs a variety of statistical and graphical operations on the concentration file(s) produced by MESOPUFF II.

The user's guide contains a brief technical description of the methods and equations. Input format specifications are given, along with detailed instructions about the use of the available options. Complete user instructions and a test case with example input/output are provided for each of these programs.

All source, receptor, and program control information is input by formatted card images. The control-paramete inputs determine which options are use in the computations and what type o output is produced.

Conclusions

A user's guide to the MESOPUFF I modeling package has been prepared. A companion report entitled "Developmen of the MESOPUFF II Dispersion Model describes the methods in detail an compares the outputs from several mode algorithms against experimental meas urements.

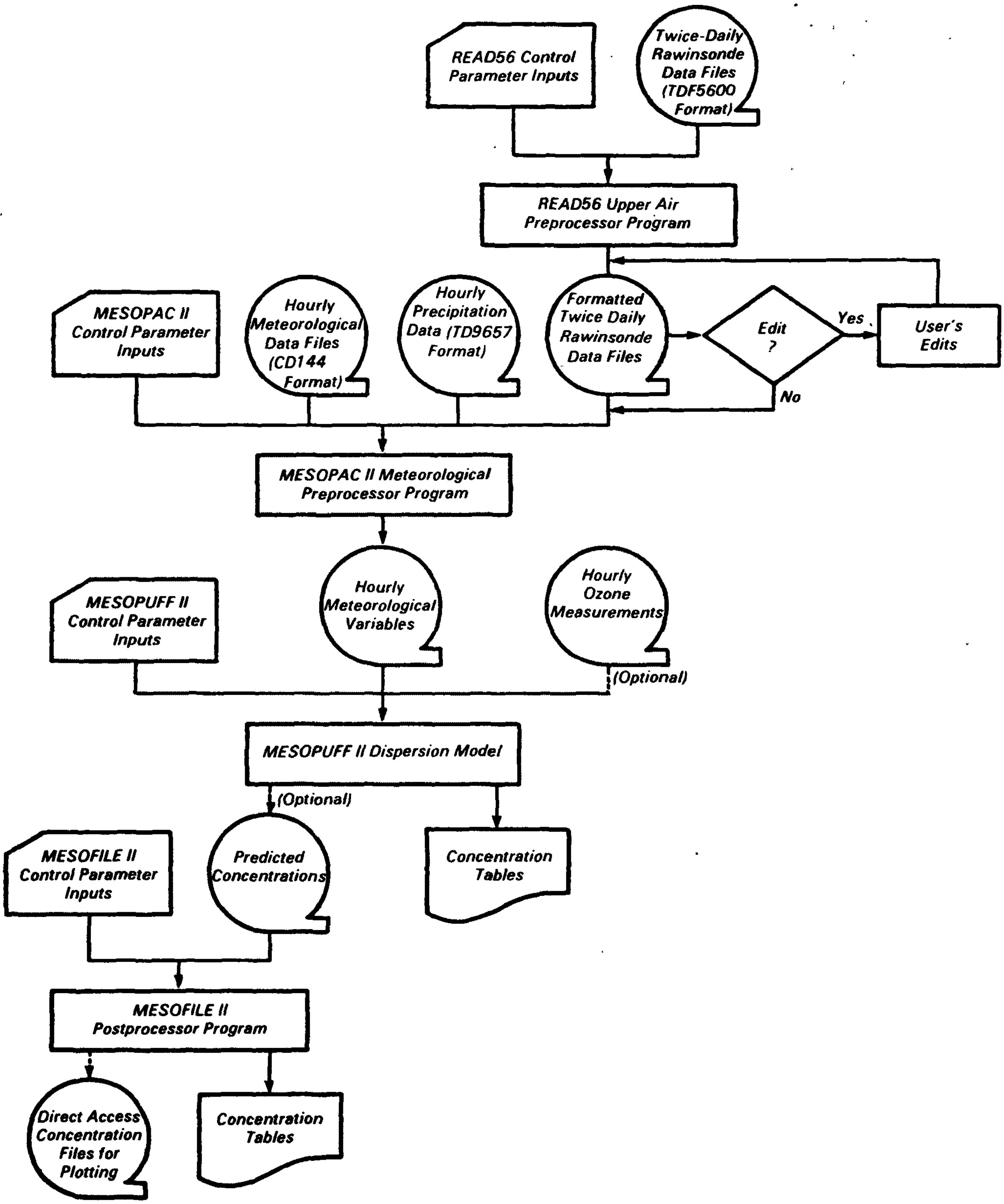

Figure 1. *MESOPUFF II modeling package.*

J. S. Scire, F. W. Lurmann, A. Bass, and S. R. Hanna are with Environmental Research and Technology, Inc., Concord, MA 01742.
***James M. Godowitch** is the EPA Project Officer (see below).*
The complete report, entitled "User's Guide to the Mesopuff II Model and Related Processor Programs," (Order No. PB 84-181 775; Cost: $20.50, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Environmental Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

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