United States Environmental Protection Agency
Research and Development

Atmospheric Sciences Research Laboratory
Research Triangle Park, NC 27711

EPA/600/S8-86/011 May 1986

EPA

Project Summary

MPDA-1: A Meteorological Processor for Diffusion Analysis — User's Guide

James Paumier, David Stinson, Terry Kelly, Catherine Bollinger, and John S. Irwin

Version 1 of the Meteorological Processor for Diffusion Analysis (MPDA-1) is a first attempt to provide a processor that can organize available meteorological data into a format accessible to diffusion analysis. MPDA-1 provides methods for preparing three types of data: National Weather Service (NWS) twice-daily radiosonde reports, NWS hourly surface observations, and user-supplied on-site data. To incorporate the surface scaling parameters, the meteorological processor is structured in accordance with current concepts of the idealized states of the planetary boundary layer. Profiles of wind velocity, temperature, and the standard deviations of vertical and lateral wind velocity fluctuations at user-specified heights are estimated.

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 availability of many diffusion models, combined with the availability of new data sources, has created a need for a processor that can organize the meteorological data into a format accessible to diffusion analyses. Version 1 of the Meteorological Processor for Diffusion Analysis (MPDA-1) is an attempt to fill this need.

Research has been conducted to obtain a better characterization of the diffusion of air pollutants and a better understanding of the meteorological variables of most concern to diffusion analyses. Most of the early popular attempts to estimate diffusion of air pollutants were based on the Gaussian-plume model. It was recognized that the only relevant measurements of wind fluctuations likely to be available for routine studies were those contained in conventional traces of horizontal wind direction. Simple rules were developed for obtaining the lateral spread, based on wind-direction trace data. In the absence of such data, the effects of thermal stratification in the lower atmosphere were represented in broad categories of stability, defined in terms of meteorological data routinely available in surface weather observations.

By the early 1970's, air quality simulation models were viewed as tools to estimate the relative magnitudes of pollutant concentration distributions from various sources, thus providing a rational basis for strategies of air quality improvement or maintenance. Most of the air quality simulation models developed in response to these modeling requirements were based on the general Gaussian-plume model. Gaussian-plume diffusion was estimated for each hour with hourly values of surface wind speed and direction, ambient air temperature, the Pasquill stability category, and mixing height. Typically, the wind direction was assumed to be constant with height. Some models provided for the variation of wind speed with height with a power-law approximation; the power-law exponent was specified as a function of Pasquill stability category. When temperature gradients were needed, as for the estimation of plume rise during stable stratification, values were assumed for each Pasquill category. It was further assumed that the diffusive characteristics of the atmosphere were vertically and horizontally homogeneous within the mixing layer.

Practical methods for characterizing the profiles of wind, temperature, and turbulence within the planetary boundary layer are now beginning to be developed. These methods are improving as new data are acquired and analyzed. In the next decade, measurement methods may develop to the point that frequent routine measurements of the structure of the planetary boundary layer may be made remotely by using Doppler-acoustic radars.

When these new methods of data acquisition are perfected, it may become possible to specify routinely the following meteorological data: mixing height, atmospheric stability, the profiles of the standard deviations of vertical and lateral wind velocity fluctuations, and the profiles of wind velocity and temperature. Availability of these data on an hourly basis has important implications for diffusion modeling. Standard deviations of wind-speed fluctuations could be used to characterize the sigmas in a Gaussian-plume model. These data would allow use of improved algorithms for estimating plume rise and for estimating wind direction shear effects, which have largely been ignored in routine modeling studies of diffusion. Also, these data would accommodate Monte-Carlo particle trajectory models of diffusion or grid models that use eddy diffusivities.

Discussion and Results

The MPDA-1 consists of a preprocessor and a meteorological processor (metprocessor), the output from which can then be used by a diffusion model. The preprocessor can accommodate data collected by standard radiosondes, surface observations, and multilevel observations at special meteorological sites (on-site observations). The preprocessor prepares and combines the data from these three sources into one unformatted file for use by the metprocessor. The metprocessor estimates the surface scaling parameters and the profile variables. A selection of methods is available for determining most meteorological parameters; these options reflect differences in the theoretical derivations of the algorithms.

Preprocessor

The preprocessor consists of a series of programs that format meteorological data according to required specifications. The preprocessor can accommodate data from three sources:

- National Weather Service (NWS) radiosondes,
- NWS surface weather observations, and
- User-provided, on-site observations

The programs in the preprocessor were developed specifically for standard NWS radiosonde and surface observation data. The data are available from the National Climatic Data Center (NCDC) in Asheville, North Carolina. The preprocessor uses radiosonde data in NCDC's TDF5600 format, and the surface observations are in the TDF1440 format.

The type of meteorological data available will dictate which programs in the preprocessor will be used. For example, if no radiosonde data are available, all of the radiosonde preprocessor routines can be skipped, but an empty file must be created for use by succeeding programs. If the user's data have already been extracted and quality-assessed, only the CONVERT programs may be needed, because they prepare the data in the format required by MERGE. The programs in the preprocessor are described briefly below.

SCAN These programs scan the tapes containing raw input data and produce a list of stations and dates recorded on the tape. The output report is not used as input to any other programs.

EXTRACT These programs extract data for the desired time period from the raw input data tapes. The user provides the range of dates of interest by specifying Julian beginning and ending dates, the station identification code, and its latitude and longitude. The specified raw data are extracted from the tapes and produced as output files.

CONVERT These programs perform two functions. 1. They reformat the output files to comply with the format specifications of the MERGE program. All programs after CONVERT use the same format. 2. They convert variables to the set of units required by the metprocessor.

QA QA programs are available for all three data types. Execution of these programs is optional. The output files created by the CONVERT programs meet the format requirements of the QA programs as well as those for MERGE. The QA programs for radiosonde and surface observation data scan the data sets for values that do not satisfy the criteria specified by the user. The QA program for on-site data gives the usei a choice between specifying acceptable ranges for all variables measured or using default values. All programs generate reports of values that do no satisfy the assessment criteria.

REDUCE Because radiosondes extenc to heights considerably greater thai those required by most diffusioi models, the reduction program delete data above a user-specified height ii each report. This routine also has a usei specified option to adjust all the height of the sounding from mean sea level t above ground level (AGL). The met processor requires heights to b specified as AGL.

HRLY-INTERP If the time interval be tween soundings is greater than on hour, this interpolation program must b used to prepare the data in the hourl format required by MERGE. The us specifies the range of dates over whic interpolation is required, and the pr gram linearly interpolates the data ov time. The output file generated contair hourly radiosonde data for the specifie date range.

MERGE MERGE combines the thr output files of the preprocess (radiosonde, surface observation, a on-site data) into one unformatt (binary) file for use by the metprocess The result is a sequence of unformatt day-records. A day-record consists one 24-h day of output, with 24 hou observations of radiosonde, surface, a on-site data.

Before executing MERGE, the three d files must be in hourly intervals a ordered sequentially by local standard ti (LST). The preprocessor can prepare a or all of the files for MERGE. However, t preprocessor does not have to be used prepare the data, as long as the forn specifications for MERGE are met. In dition to the unformatted output file u by the metprocessor, MERGE will a generate a formatted output file if the u requests it.

Metprocessor

The metprocessor uses data combi by MERGE to calculate the meteorolog parameters required by diffusion models. Estimates of the fundamental surface scaling parameters (including surface fluxes and Monin-Obukhov length), surface roughness length, and mixing height are determined first. This is followed by estimates of wind velocity, temperature, and standard deviations of the horizontal and vertical wind speed fluctuations at heights specified by the user. Methods are available that require only NWS radiosonde and surface observation data to estimate all the variables. Other methods are available that incorporate on-site data to estimate variables.

The metprocessor consists of a main program and a series of subroutines that calculate the individual parameters and construct profiles.

The user's choices for a method of calculation for each of the parameters and profiles are listed in Table 1. Each method is encoded as a separate subroutine.

The metprocessor processes one day-record (24-h record) from MERGE at a time. All data are in local standard time. Because processing is day-by-day, information from the previous day is unavailable for computation during the current day. This limitation must be considered if the user adds additional subroutines.

Conclusions and Recommendations

MPDA-1 offers a set of methods for preparing three types of data for use in diffusion analysis: NWS twice-daily radiosonde reports, NWS hourly surface weather observations, and user-supplied on-site data. A selection of methods is available for estimating vertical profiles of wind velocity and temperature and the standard deviations of vertical and lateral wind velocity fluctuations. Procedures are also provided for estimating mixing height and surface scaling parameters, including the Monin-Obukhov length.

The main feature of MPDA-1 is its flexible design, which will allow easy adaptation to new processing methods and new diffusion models. This is true also for the preprocessor portion of the system. Each method for calculating a parameter or profile is a separate subroutine; the modular design adapts easily to changes in input data formats. The modular design is also used in the preprocessor.

Because each method computes only one surface parameter or constructs a profile, the user can easily add an alternative method for a parameter and use it in the computations, rather than one supplied with the system. The user is encouraged to submit any subroutines or algorithms that demonstrate improved accuracy or speed. The part of the preprocessor concerned with on-site data contains several variables that are not used in the MPDA-1. These variables are thus available to the user who develops his own metprocessor algorithms. The MPDA is a continually evolving system; user comments and suggestions are welcome.

MPDA-1 was developed with specific design criteria in mind. These criteria and the methods by which they were met are listed in Table 2. The criteria reflect the goal of creating a system with as much built-in flexibility as possible.

At least one method for each parameter is provided, so that the system can be used even if only NWS upper air data and surface observations are available. The upper air data used during development of MPDA-1 were from NWS radiosondes collected at 0000 Greenwich Mean Time (GMT) and 1200 GMT. Because the MPDA-1 metprocessor requires hourly data, the soundings are interpolated to hourly values. Adding on-site data from multilevel instrumented towers or remote sensors would expand the number of usable methods available and improve the results for the lower part of the atmosphere.

As with any system, the MPDA-1 does have limitations. The system is easy to implement, but the user should note that certain methods require more sophisticated input data than are typically available in a routine weather observation. The user should specify methods that are compatible with the data available. For example, if on-site data are not available, then some of the methods cannot be fully utilized.

With these limitations in mind, the user will find the MPDA-1 to be a flexible and effective system for organizing meteorological data into a format accessible to diffusion analyses.

Table 1. Choices of Subroutines Containing Methods of Calculation for Parameters and Profiles in the Metprocessor

Parameter or Profile	Subroutine Name	Description
Surface roughness length, z_0 (m)	ZOMOD1	Roughness length estimated from user-defined land-use and terrain types.
	ZOMOD2	User-specified value, or if unavailable, a default value of 0.3 m.
Surface heat flux, H_0 (W/m^2) and Surface friction velocity, u^* (m/s)	HMOD1 and USMOD1	Heat flux estimated using surface layer similarity theory and low-level profile data of wind speed and temperature difference.
	HMOD3 and USMOD3	Parameterization of surface energy fluxes in terms of standard weather observations of cloud cover, temperature, and near-surface wind speed and surface roughness length (z_0).
	HMOD4 and USMOD4	User-supplied values from on-site data. If an hourly value is missing, the method defaults to HMOD3/USMOD3.
Monin-Obukhov length (m)	LMOD2	Direct computation using H_0 and u^*
Convectively driven mixing height (m)	ZCMOD1	Rate equation for a zero-order jump model coupled with a free convection formula.
	ZCMOD2	Intersection of the sunrise radiosonde report with the dry adiabat corresponding to the hourly surface temperature.
	ZCMOD3	User-supplied value from on-site data. If an hourly value is missing, the method defaults to ZCMOD1.
Mechanically driven mixing height (m)	ZMMOD1	$z_m \propto u^*/f$, where f is the Coriolis parameter.
	ZMMOD2	Daytime: $z_m \propto u^*/f$ Nighttime: $z_m \propto (u^*/f)/(1 + 1.9z_m/L)$
	ZMMOD3	User-supplied value from on-site data. If an hourly value is missing, the method defaults to ZMMOD2.
Heights (m)	HTMOD1	User-specified.
	HTMOD2	User-supplied fractions of mixing height.
Temperature profile (°C)	TMOD1	Assumes constant potential temperature below the daytime convective mixing height: below the nighttime surface-based inversion height, potential temperature $\propto (1 - z/h_i)^3$.
Wind velocity profile (m/s)	UVMOD2	Weighted average of wind velocity profiles estimated from similarity theory and determined from radiosonde reports.
	UVMOD3	Interpolated from user-supplied wind profile data. When data are missing or insufficient, the method defaults to UVMOD2.
	UVMOD4	Same as UVMOD2, except that linear weighting functions are used. The weights for wind speed and wind direction are treated separately.
Vertical and horizontal wind velocity fluctuations (variances) (m/s)	SWMOD1 and SVMOD1	Estimated from empirical parameterizations using h_m, u^*, and convective scaling velocity.
	SWMOD2 and SVMOD2	On-site values of the variances are used as correction factors to estimates made by SWMOD1 and SVMOD1.

Table 2. Design Criteria for the Metprocessor

Need	Implementation
— New methods must be easily added: obsolete methods must be easily deleted.	— The computations associated with each method occur within individual subroutines: to add or delete a method, only a change in the main program is needed.
— The input data and results from computations must be readily accessible.	— The data are accessible to all subroutines in their entirety via COMMON blocks.
— The code must be standard for most computer systems.	— ANSI FORTRAN 77 was used to code the system.
— Must be able to vary output by parameters and style, depending on the requirements of the diffusion model.	— Output is generated by subroutines: thus, new output styles or variable lists can be easily added by adding subroutines.

☆U. S. GOVERNMENT PRINTING OFFICE: 1986/646-116/20837

James Paumier, David Stinson, Terry Kelly, and Catherine Bollinger are with Computer Sciences Corporation, Research Triangle Park, NC 27709; the EPA author ***John S. Irwin*** *is with the Atmospheric Sciences Research Laboratory, Research Triangle Park, NC 27711.*
D. Bruce Turner *is the EPA Project Officer (see below).*
The complete report, entitled "MPDA-1: A Meteorological Processor for Diffusion Analysis—User's Guide," (Order No. PB 86-171 402/AS; Cost: $16.95, 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:
Atmospheric Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

Official Business
Penalty for Private Use $300

EPA/600/S8-86/011

0000329 PS

U S ENVIR PROTECTION AGENCY
REGION 5 LIBRARY
230 S DEARBORN STREET
CHICAGO IL 60604