US EPA's Guidelines for Air Quality Models

APPENDIX B TO APPENDIX W OF PART 51 -- SUMMARIES OF ALTERNATIVE AIR QUALITY MODELS

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B.0 INTRODUCTION AND AVAILABILITY

This appendix summarizes key features of refined air quality models that may be considered on a case-by-case basis for individual regulatory applications. For each model, information is provided on availability, approximate cost, regulatory use, data input, output format and options, simulation of atmospheric physics and accuracy. The models are listed by name in alphabetical order.

There are three separate conditions under which these models will normally be approved for use:

1. A demonstration can be made that the model produces concentration estimates equivalent to the estimates obtained using a preferred model (e.g., the maximum or high, second-high concentration is within 2% of the estimate using the comparable preferred model);

2. A statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the model in Appendix B performs better for the application than a comparable model in Appendix A; and

3. There is no preferred model for the specific application but a refined model is needed to satisfy regulatory requirements.

Any one of these three separate conditions may warrant use of these models. See Section 3.2, Use of Alternative Models, for additional details.

Many of these models have been subject to a performance evaluation by comparison with observed air quality data. A summary of such comparisons for models contained in this appendix is included in Moore *et al.* (1982). Where possible, several of the models contained herein have been subjected to rigorous evaluation exercises, including (l) statistical performance measures recommended by the American Meteorological Society and (2) peer scientific reviews.

A source for some of these models and user's documentation is Computer Products, National Technical Information Service (NTIS), U.S. Department of Commerce, Springfield, VA 22161, Phone: (703) 487-4650. A number of the model codes and selected, abridged user's guides are also available from the Support Center for Regulatory Air Models Bulletin Board System[19] (SCRAM BBS), Telephone (919) 541-5742. The SCRAM BBS is an electronic bulletin board system designed to be user friendly and accessible from anywhere in the country. Model users with personal computers are encouraged to use the SCRAM BBS to download current model codes and text files.

B.5 HOTMAC/RAPTAD

Reference

Mellor, G.L. and T. Yamada, 1974. A Hierarchy of Turbulence Closure Models for Planetary Boundary Layers. *Journal of Atmospheric Sciences,* 31: 1791-1806.

Mellor, G.L. and T. Yamada, 1982. Development of a Turbulence Closure Model for Geophysical Fluid Problems. *Rev. Geophys. Space Phys.,* 20: 851-875.

Yamada, T. and S. Bunker, 1988. Development of a Nested Grid, Second Moment Turbulence Closure Model and Application to the 1982 ASCOT Brush Creek Data Simulation. *Journal of Applied Meteorology,* 27: 562-578.

Availability

For a cost to be negotiated with the model developer, a 1/4 - inch data cartridge or a 4mm DAT tape containing the HOTMAC® /RAPTAD® computer codes including pre- and post-processors and hard copies of user manuals (User's Manual, Maintenance Manual, Operations Manual, Maintenance Interface Manual, Topo Manual, and 3-Dimensional Plume Manual) are available from YSA Corporation, Rt. 4 Box 81-A, Santa Fe, NM 87501; Phone: (505) 989-7351; Fax: (505) 989-7965; e-mail: ~~ysa@RT66.com~~ ysa@ysasoft.com

Abstract

YSA Corporation offers a comprehensive modeling system for environmental studies. The system includes a mesoscale meteorological code, a transport and diffusion code, and extensive Graphical User Interfaces (GUIs). This system is unique because the diffusion code uses time dependent, three-dimensional winds and turbulence distributions that are forecasted by a mesoscale weather prediction model. Consequently the predicted concentration distributions are more accurate than those predicted by traditional models when surface conditions are heterogeneous. In general, the modeled concentration distributions are not Gaussian because winds and turbulence distributions change considerably in time and space over complex terrain.

The models were originally developed by using super computers. However, recent advancement of computer hardware has made it possible to run complex three-dimensional meteorological models on desktop workstations. The present versions of the programs are running on super computers and workstations. GUIs are available on Sun Microsystems and Silicon Graphics workstations. The modeling system can also run on a laptop workstation, which makes it possible to run the programs in the field or away from the office. As technology continues to advance, a version of HOTMAC®/RAPTAD® suitable for PC-based platforms will be considered for release by YSA.

HOTMAC®, Higher Order Turbulence Model for Atmospheric Circulation, is a mesoscale weather prediction model that forecasts wind, temperature, humidity, and atmospheric turbulence distributions over complex surface conditions. HOTMAC® has options to include non-hydrostatic pressure computation, nested grids, land-use distributions, cloud, fog, and precipitation physics. HOTMAC® can interface with tower, rawinsonde, and large-scale weather data using a four-dimensional data assimilation method. RAPTAD®, Random Puff Transport and Diffusion, is a Lagrangian random puff model that is used to forecast transport and diffusion of airborne materials over complex terrain. Concentrations are computed by summing the concentration of each puff at the receptor location. The random puff method is equivalent to the random particle method with a Gaussian kernel for particle distribution. The advantage of the puff method is the accuracy and speed of computation. The particle method requires the release of a large number of particles, which could be computationally expensive. The puff method requires the release of a much less number of puffs, typically 1/10 to 1/100 of the number of particles required by the particle method.

The averaging time for concentration estimates is variable from 5 minutes to 15 minutes for each receptor. In addition to the concentration computation at the receptor sites, RAPTAD® computes and graphically displays hourly concentration contours at the ground level. RAPTAD® is applicable to point and area sources.

The meteorological data produced from HOTMAC® are used as input to RAPTAD®. RAPTAD® can forecast concentration distributions for neutrally buoyant gas, buoyant gas and denser-than-air gas. The models are significantly advanced in both their model physics and in their operational procedures. GUIs are provided to help the user prepare input files, run programs, and display the modeled results graphically in three dimensions.

a. Recommendation for Regulatory Use

There are no specific recommendations at the present time. The HOTMAC® /RAPTAD® modeling system may be used on a case-by-case basis.

b. Input Requirements

Meteorological Data: The modeling system is significantly different from the majority of regulatory models in terms of how meteorological data are provided and used in concentration simulations. Regulatory models use the wind data, which are obtained directly from measurements or analyzed, by using a simple constraint such as a mass conservation equation. Thus, the accuracy of the computation will depend significantly on the quantity and quality of the wind data. This approach is acceptable as long as the study area is flat and the simulation period is short. As the regulations become more stringent and more realistic surface conditions are required, a significantly large volume of meteorological data is required which could become very expensive.

An alternative approach is to augment the measurements with predicted values from a mesoscale meteorological model. This is the approach we have taken here. This approach has several advantages over the conventional method. First, concentration computations use the model forecast wind while the conventional method extrapolates the observed winds. Extrapolation of wind data over complex terrain and for an extended period of time quickly loses its accuracy. Secondly, the number of stations for upper air soundings is typically limited from none to at most a few stations in the study area. The corresponding number in a mesoscale model is the number of grid points in the horizontal plane which is typically 50 X 50. Consequently, concentration distributions using model forecasted winds would be much more accurate than those obtained by using winds, which were extrapolated from the limited number of measurements.

HOTMAC® requires meteorological data for initialization and to provide boundary conditions if the boundary conditions change significantly with time. The minimum amount of data required to run HOTMAC® is wind and potential temperature profiles at a single station. HOTMAC® forecasts wind and turbulence distributions in the boundary layer through a set of model equations for solar radiation, heat energy balance at the ground, conservation of momentum, conservation of internal energy, and conservation of mass.

Terrain Data: HOTMAC® and RAPTAD® use the digitized terrain data from the U.S. Geological Survey and the Defense Mapping Agency. Extraction of terrain data is greatly simplified by using YSA's GUI software called Topo. The user specifies the latitudes and longitudes of the southwest and north east corner points of the study area. Then, Topo extracts the digitized elevation data within the area specified and converts from the latitudes and longitudes to the UTM (Universal Transverse Mercator) coordinates for up to three nested grids.

Emission Data: Emission data requirements are emission rate, stack height, stack diameter, stack location, stack gas exit velocity, and stack buoyancy.

Receptor Data: Receptor data requirements are names, location coordinates, and desired averaging time for concentration estimates, which is variable from 5 to 15 minutes.

c. Output

HOTMAC® outputs include hourly winds, temperatures, and turbulence variables at every grid point. Ancillary codes graphically display vertical profiles of wind, temperature, and turbulence variables at selected locations and wind vector distributions at specified heights above the ground. These codes also produce graphic files of wind direction projected on vertical cross sections.

RAPTAD® outputs include hourly values of surface concentration, time variations of mean and standard deviation of concentrations at selected locations, and coordinates of puff center locations. Ancillary codes produce color contour plots of surface concentration, time variations of mean concentrations and ratios of standard deviation to mean value at selected locations, and concentration distributions in the vertical cross sections. The averaging time of concentration at a receptor location is variable from 5 to 15 minutes. Color contour plots of surface concentration can be animated on the monitor to review time variations of high concentration areas.

d. Type of Model

HOTMAC® is a 3-dimensional Eulerian model for weather forecasting, and RAPTAD is a 3-dimensional Lagrangian random puff model for pollutant transport and diffusion.

e. Pollutant types

RAPTAD® may be used to model any inert pollutants, including dense and buoyant gases.

f. Source-Receptor Relationship

Up to six point or area sources are specified and up to 50 sampling locations are selected. Source and receptor heights are specified by the user.

g. Plume Behavior

Neutrally buoyant plumes are transported by mean and turbulence winds that are modeled by HOTMAC. Non-neutrally buoyant plume equations are based on Van Dop (1992). In general, plumes are non-Gaussian.

h. Horizontal Winds

RAPTAD® uses wind speed, wind direction, and turbulence on a gridded array that is supplied hourly by HOTMAC®. Stability effect and mixed layer height are incorporated through the intensity of turbulence, which is a function of stability. HOTMAC® predicts turbulence intensity by solving a turbulence kinetic energy equation and a length scale equation. RAPTAD® interpolates winds and turbulence at puff center locations every 10 seconds from the values on a gridd
ed array. RAPTAD® can also use the winds observed at towers and by rawinsondes.

i. Vertical Wind Speed

RAPTAD® uses vertical winds on a gridded array that are supplied hourly by HOTMAC®. HOTMAC® computes vertical wind either by solving an equation of motion for the vertical wind or a mass conservation equation. RAPTAD® interpolates vertical winds at puff center locations every 10 seconds from the values on a gridded array.

j. Horizontal Dispersion

Horizontal dispersion is based on the standard deviations of horizontal winds that are computed by HOTMAC®.

k. Vertical Dispersion

Vertical dispersion is based on the standard deviations of vertical wind that are computed by HOTMAC®.

l. Chemical Transformation

HOTMAC® can provide meteorological inputs to other models that handle chemical reactions, e.g., UAM.

m. Physical Removal

Not treated.

n. Evaluation Studies

Yamada, T., S. Bunker and M. Moss, 1992. A Numerical Simulation of Atmospheric Transport and Diffusion over Coastal Complex Terrain. *Journal of Applied Meteorology,* 31: 565-578.

Yamada, T. and T. Henmi, 1994. HOTMAC: Model Performance Evaluation by Using Project WIND Phase I and II Data. Mesoscale Modeling of the Atmosphere, American Meteorological Society, Monograph 47, pp. 123-135.