

# Comprehensive Modeling System for Atmospheric Transport and Diffusion

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## I. Introduction

Conventional models used for atmospheric transport and diffusion studies assume that the wind field over the geographical area of interest can be adequately represented by the wind speed and direction over a single site. These models also assume that the plume or puff released to the atmosphere is symmetrically distributed (e.g. Gaussian distribution) around a centerline that originates at the point of release and proceeds in one direction. The transport direction is determined from the wind direction measured at the single observation site. While the above assumptions may be acceptable in the homogeneous topography case, however, a single value or a single profile of wind cannot provide realistic wind distribution for accurate transport and diffusion computations over complex terrain. Therefore, more accurate predictive system is required for realistic terrain and meteorological conditions.

YSA Corporation offers a comprehensive modeling system for atmospheric transport and diffusion for environment studies, which includes a 3-D mesoscale meteorological code (HOTMAC) and a 3-D Lagrangian transport and diffusion code (RAPTAD). This system is unique because the diffusion code uses time dependent, three-dimensional winds and turbulence distributions produced by the mesoscale weather prediction model. Consequently the predicted concentration distributions are more accurate than those predicted by traditional models when surface conditions are heterogeneous. The modeled concentration distributions are not Gaussian because winds and turbulence distributions change considerably in time and space over complex terrain. HOTMAC and RAPTAD are listed in the EPA's "Guidelines for Air Quality Models", Appendix B.

## II. Key components

- **HOTMAC**

HOTMAC, Higher Order Turbulence Model for Atmospheric Circulation (Yamada and Bunker 1988), is a 3-D mesoscale weather prediction model that forecasts

wind, temperature, humidity, and atmospheric turbulence distribution over complex surface conditions. The model's closure hypotheses that relate unknown higher-order moments to the known lower-order moments are based on the work by Mellor and Yamada (1974, 1982).

The governing equations are conservation equations for mass, momentum, potential temperature deviations from area average, water vapor, and turbulence kinetic energy. A terrain-following vertical coordinate system is used in order to increase the accuracy in the treatment of surface boundary condition. The surface boundary conditions are obtained by applying a heat energy balance at the surface. Both long-wave and short-wave radiation parameterizations are considered in the model. HOTMAC has options to include non-hydrostatic pressure computation, land-use distributions, and precipitation physics. HOTMAC can interface with radar profiler, rawinsonde, and large-scale weather data using a four-dimensional data assimilation method.

A typical grid is  $40 \times 40 \times 16$  and nested region uses  $25 \times 25 \times 16$  grid points. The 3-D grid configurations can be easily changed by users. Horizontal grid spacing from a few hundred meters to over 20km have been used. An alternating-direction-implicit finite-differencing technique is used for time integration and a time step is chosen to satisfy Courant-Friedrich-Lewy criteria. In order to increase the accuracy of finite-difference approximation, mean and turbulence variables are defined at grids which are staggered both in horizontal and vertical directions.

#### • RAPTAD

RAPTAD, Random Puff Transport and Diffusion (Yamada 1985), is a 3-D Lagrangian random puff model that is used to forecast transport and diffusion of airborne materials over complex terrain. Puffs are released at the source and the change of puff characteristics with time, such as the location of the center, and the size and age of the puff are computed every time step. The meteorological data produced from HOTMAC are used as input to RAPTAD.

The concentration level at a given time and space is calculated as the sum of the concentrations from each puff at the receptor location. Various functional forms can be assumed to express the concentration distribution in the puff. A Gaussian distribution is used where variances are determined as the time integration of the velocity variances which is encountered over the history of the puff.

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.

RAPTAD can forecast concentration distributions for neutrally buoyant gas, buoyant gas and denser-than-air gas. For nonneutrally buoyant plume, plume's vertical velocity and temperature are computed by the Langevin equation (Van Dop 1992). RAPTAD is applicable to point and area sources. RAPTAD uses graphical user interfaces to interact with user.

This modeling system was originally developed for research purposes and ran on super computers. However, recent advancement of computer hardware has made it possible to run complex 3-D meteorological models on desktop workstations and PCs. HOTMAC/RAPTAD runs on super computers, workstations and PCs. It can also run on a laptop workstation which make it possible to run the programs in the field or away from the office. Comprehensive graphical user interfaces (GUIs) make the software easy to use with a short learning curve.

### **III. Auxiliary Components**

#### **• TOPO**

TOPO is a data pre-processor which is used to generate input parameters for HOTMAC. The models, HOTMAC and RAPTAD, use the digitized terrain data from the U. S. Geological Survey and the Defense Mapping Agency. TOPO's user friendly interface greatly simplifies terrain data extraction and allows user to select up to three nested grids. The user specifies the latitudes and longitudes of the southwest and northeast corner points of the study area. Then, TOPO extracts the digitized elevation data within the area specified and converts the latitudes and longitudes to the UTM (Universal Transverse Mercator) coordinates.

#### **• LSM2HOT**

The LSM2HOT is a data pre-processor which allows user to extract largescale meteorological data from various data sources and converts to HOTMAC input format. The largescale meteorological variables are first interpolated vertically at the HOTMAC heights at the original locations and then interpolated horizontally at the HOTMAC horizontal grid locations. LSM2HOT also use graphical user interfaces to interact with user.

#### **• Graphics**

YSA has developed scientific visualization programs exclusively for displaying HOTMAC and RAPTAD outputs. These programs are written by using NCAR Graphics software package and embedded in each component of the GUIs. These programs produce variety of plots such as vertical profiles, wind vector distributions, concentration contours, cross-section plots, concentration versus time, and three-dimensional rendering. These plots are displayed on the screen and may be saved to create a video animation,

presentations, etc. GUIs simplify greatly these post-processing procedures to a level of mouse clicks.

#### **IV. Applications**

This model system has been used internationally for various environmental studies. Its application includes: emergency-response management associated with accidental release of toxic materials, environmental assessment for city and industrial site planning, decision-making in weather-influenced field operations, and atmospheric boundary-layer research. Some examples of the model applications will be presented in the meeting.

#### **V. References**

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