QC
807.5
.U6
A7
no.195
c.2

NOAA Technical Memorandum ERL ARL-195

HYBRID SINGLE-PARTICLE LAGRANGIAN INTEGRATED TRAJECTORIES (HY-SPLIT): VERSION 3.0 - - USER'S GUIDE AND MODEL DESCRIPTION

Roland R. Draxler

Air Resources Laboratory
Silver Spring, Maryland
June 1992

noaa NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION / Environmental Research Laboratories

QC
807.5
.U6
A7
No.195
c.2

NOAA Technical Memorandum ERL ARL-195

HYBRID SINGLE-PARTICLE LAGRANGIAN INTEGRATED TRAJECTORIES (HY-SPLIT): VERSION 3.0 - - USER'S GUIDE AND MODEL DESCRIPTION

Roland R. Draxler

LIBRARY
SEP 0 9 1992
N.O.A.A.
U.S. Dept. of Commerce

Air Resources Laboratory
Silver Spring, Maryland
June 1992

UNITED STATES
DEPARTMENT OF COMMERCE

Barbara Hackman Franklin
Secretary

NATIONAL OCEANIC AND
ATMOSPHERIC ADMINISTRATION

John A. Knauss
Under Secretary for Oceans
and Atmosphere/Administrator

Environmental Research
Laboratories

Joseph O. Fletcher
Director

NOTICE

Mention of a commercial company or product does not constitute an endorsement by NOAA Environmental Research Laboratories. Use of information from this publication concerning proprietary products or the tests of such products for publicity or advertising purposes is not authorized.

For sale by the National Technical Information Service, 5285 Port Royal Road
Springfield, VA 22161

CONTENTS

Page

ABSTRACT

1. INTRODUCTION 1

1.1. Modeling system overview 1

1.2 Validation Studies 2

2. PROGRAM AND FILE STRUCTURE 4

2.1 Pre-processors 5

2.2 Transport and Dispersion 9

2.3 Post-Processing 11

3. METEOROLOGICAL DATA 12

3.1 Upper Air and Surface Observations 13

3.2 NMC Gridded Archive and Forecast Data 14

3.3 Special Observational Data 15

3.4 Data Archive Management 15

4. HY-SPLIT OUTPUT OPTIONS 17

4.1 Run-time Displays 18

4.2 Post-processing Displays 20

5. SPECIAL EXAMPLES 22

5.1 Backward Trajectories 22

5.2 Vertical Motion 23

6. MISCELLANEOUS APPLICATIONS 23

6.1 Multiple Source Emissions 23

6.2 Sulfur Chemistry 24

6.3 Nitrogen Chemistry 24

6.4 Particles, Deposition, and Decay 24

6.5 Radiological Routines 24

7. ACKNOWLEDGMENTS 25

8. REFERENCES 25

Appendix A - Transport and Dispersion

Appendix B - HY-SPLIT Meteorological Processor

Appendix C - Rawinsonde Data Preprocessor

Appendix D - Gridded Meteorological Data Format

Appendix E - Default.Dat Input File Description

Appendix F - Default.CFG Input File Description

Appendix G - Installation, Running, and File Formats

Appendix H - HYTEK Tektronix Terminal Emulator

Appendix I - HY-SPLIT Error Codes

Appendix J - Verification Studies

List of Tables

		Page
1.	Modeling system flowchart	5

List of Tables - Appendices

1C.	Functions for normalized profiles of momentum and heat	C.2
1D.	Structure and orientation of meteorological data grids	D.1
2D.	Availability of meteorological data	D.3
3D.	Meteorological parameters and their organization	D.4
4D.	Vertical levels available in each data set	D.5
5D.	Grid structure of packaged data	D.6
1J.	Statistical summary of ANATEX simulations	J.2

List of Figures

		Page
1	Sample display for the base case (test001) from the HYEDIT program.	6
2	Sample display from the HYPICK default.dat mouse based file editor.	7
3	Sample display from the HYMAPS default.dat file mouse based editor program.	8
4	Illustration of the ASCII screen display during a model simulation without run-time graphics (test001).	10
5	A snapshot map from a single release (test002) after 24th travel.	18
6	Trajectory map after 24-h travel time with positions shown hourly (test003).	19
7	Run-time concentration map display (test004) showing the 24-h average values.	20
8	Postprocessing trajectory output from TRAJPLOT (test005) is identical to that shown in Fig. 6.	20
9	Illustration from qualitative concentration display (test006).	21
10	Illustration from the quantitative concentration display.	21
11	Backward trajectory computation (test007) for the forward case shown in Fig. 6.	22
12	Trajectory with vertical velocity computed from the divergence field (test008).	23

List of Figures - Appendices

		Page
1A	Normal probability distribution. The dashed horizontal line indicates the ordinate value at which the shaded area equals the area above the line at 1.54 σ.	A-3
2A	The distance (A) a particle is advected during a time step. Three positions are interpolated so that the concentrations can be computed at all grid points at the interpolated (dashed) and initial and final positions (solid).	A-4
3A	Illustration of how a single particle Q0 splits due to vertical diffusion into two particle Q2 and Q3.	A-5
4A	Illustration of how a single particle with radius R splits due to horizontal diffusion into four particles each with radius R/2.	A-5
5A	Illustration of when two particles are merged into a single particle. It occurs when the difference between the vectors is less than R.	A-6
1D	NGM data grid number 6.	D-2
2D	MRF northern hemisphere data grid number 2.	D-2
3D	MRF southern hemisphere data grid number 3.	D-2
1J	Three-month average measured concentration for releases from both Glasgow and St. Cloud.	J-1
2J	Three-month average calculated concentration for release from Glasgow and St. Cloud.	J-1
3J	Average measured concentration (fl/L) from all CAPTEX releases.	J-3
4J	Average calculated concentration from all the CAPTEX tracer releases.	J-3
5J	The ratio of calculated to measured concentration pairs sorted by cumulative percent for the CAPTEX and ANATEX experiments.	J-4
6J	Trajectory using MRF data, comparable to the case shown with NGM data in simulation test005.	J-5
7J	Air concentration estimates using MRF data, similar to the NGM case shown in Fig. 10 (test006).	J-6

HYBRID SINGLE-PARTICLE LAGRANGIAN INTEGRATED TRAJECTORIES (HY-SPLIT): VERSION 3.0 -- USER'S GUIDE AND MODEL DESCRIPTION

Roland R. Draxler

ABSTRACT. The algorithms and equations used in the calculation of long-range pollutant transport and dispersion are presented from the meteorological data sources through the calculation of air concentrations. The model calculation methods are a hybrid between Eulerian and Lagrangian approaches. A single pollutant particle represents the initial source. Advection and diffusion calculations are made in a Lagrangian framework. However, meteorological input data can either be gridded from rawinsonde observations or archived from other sources, such as the analyses fields or forecast outputs from Eulerian primitive equation models. As the dispersion of the initial particle spreads it into regions of different wind direction or speed, the single particle is divided into multiple particles to provide a more accurate representation of the complex flow field. Air concentrations are calculated on a fixed three dimensional grid by integrating all particle masses over the sampling time. The model code can be run on a personal computer. Calculations consist of simple trajectories from a single source to complex multiple source emissions. A flow chart of the calculations as well as several examples are given. The code is structured so that concentration calculations or simple trajectory (forward or backward) calculations can be performed on sigma (terrain following) or pressure coordinates.

1. INTRODUCTION

1.1 Modeling System Overview

The development of the HY-SPLIT long-range transport calculation technique has evolved in several stages, from a simple wind-shear induced particle dispersion study (Draxler and Taylor, 1982), to the inclusion of air concentration calculations with only a day/night mixing assumption (Draxler, 1982), to the calculation of vertical mixing coefficient profiles and vertical particle motions (Draxler, 1987). The modeling technique has many similarities to particle-in-cell (PIC) methods (Lange, 1978) with the primary exception that one starts with only a single particle that may split into as many particles as needed to describe the pollutant distribution. This approach requires special numerical techniques to limit the number of particles. The equations and calculational methods are discussed in much more detail in Appendix A.

Although each particle has an associated horizontal and vertical diffusive component, similar to a "puff" model, the subsequent particle divisions determine the spatial and temporal concentration distributions, rather than the diffusion about any one particle. With PIC methods the initial concentration distribution is defined by the distribution of particles, but at later times there may be too few particles in adjacent cells to define the concentration field without assuming a particle probability distribution. In contrast with HY-SPLIT, near the source region, the concentrations are most sensitive to the assumed distribution about the single emitted particle, while at further downwind distances the concentrations are most sensitive to the subsequent particle distribution.

In most transport and dispersion models, the limiting feature to the accuracy of the calculations is the spatial and temporal resolution of the meteorological data. In previous model versions rawinsonde observations, with limited spatial (400 km) and temporal density (every 12 hr), were the only data source. The rawinsonde data were then gridded on a user-selected polar stereographic grid by a preprocessor program (see Appendix C). This was the method used when the dispersion model calculations were compared with the air concentrations measured during the Cross Appalachian Tracer Experiment (CAPTEX) (Draxler, 1987; Draxler and Stunder, 1988). The current HY-SPLIT version permits the use of meteorological input data from other sources, in particular meteorological data fields archived from the National Meteorological Center's (NMC) Nested Grid Model (NGM - Phillips, 1975) over the continental U.S. (90 to 180 km every 1 to 2 hr) or data archived from the initialization fields of NMC's Medium Range Forecast Model (MRF) for global coverage (381 km every 6 h). These data are discussed in much more detail in Appendix D. An explanation of how the HY-SPLIT code converts the different data sources into a common structure can be found in Appendix B.

1.2 Validation Studies

One of the more important aspects of any transport and dispersion code is understanding the causes of uncertainty and the potential errors in the resulting calculations. A major long-range validation experiment was conducted during January through March of 1987, Across North America Tracer Experiment (ANATEX - see Draxler et al., 1991). Inert tracers were released from two sources routinely every 2½ days and daily averaged samples were collected at distances of up to 3000 km from the tracer sources. Enhanced 4 per day rawinsonde observations as well as high resolution NGM model output were available for the three month experimental period. A detailed evaluation of several long-range transport models, including HY-SPLIT, using the ANATEX data was conducted by Clark and Cohn (1990).

Other validation studies during ANATEX (Draxler, 1990) compared the NGM data with meteorological observations on a 500 m tower. The results showed that on average the NGM accurately predicted the diurnal variations of wind, temperatures, and mixing. One result from that study was the incorporation of an Ekman/similarity wind interpolation module within HY-SPLIT to calculate the wind profiles at levels below the lowest sigma level (about 180 m) available from the NGM. Another conclusion was that it is not possible to interpolate

the diurnal cycle of vertical mixing from only two observations per day.

Trajectory accuracy from calculations using HY-SPLIT during the ANATEX period was estimated (Draxler, 1991) from back trajectories calculated from aircraft observations of the tracer plume position. Transport distances varied from about 50 to 300 km from the source and calculations were performed using rawinsonde data (4 per day) and high resolution NGM data (90 km every 2 h). In the 30 trials with aircraft observations, no significant difference was discernable in trajectory accuracy of calculations using the different meteorological input data. Trajectory error ranged from 20% to 30% of the travel distance. When trajectories were grouped into similar categories, the NGM data provided the best results when smaller scale flow features were present--ones that could not be resolved in the rawinsonde network. The 4 per day rawinsonde data provided the best results when fronts or low pressure systems were present in the vicinity of the tracer release. Slower transport in more homogeneous zonal flow regimes resulted in some of the smallest errors of around 15% of the travel distance. One general conclusion was that the NGM generated initialization and forecast data was an adequate substitute for 4 per day rawinsonde observations in trajectory calculations.

High resolution temporal and spatial meteorological data are not always available when the data source is from the MRF. The effect of lower resolution data on trajectory accuracy (Rolph and Draxler, 1990) was tested during the ANATEX period by degrading the high resolution NGM data in space and time and calculating the difference in those trajectories from the base case calculated with the high resolution data (90 km every 2 h). Transport times of 96 h, using 90 km data every 4 h, resulted in an error of 8% in contrast to an error of 5% when the data were maintained at 2 h intervals but reduced to 180 km resolution. These errors are relative to the base case, which as was discussed in the previous paragraph can be much larger. Essentially the NGM data were initially most sensitive to temporal frequency rather than spatial resolution. This resulted in a decision to archive the NGM model output at every other grid point, 180 km, but at 2 h intervals, primarily to maintain the highest level of accuracy, while still keeping the data archive as compact as possible. When the NGM data were degraded to 360 km at 6 h intervals, comparable to the MRF archive data, the relative trajectory error after 96 h was about 17%. Assuming from the previous aircraft validation study that the average absolute trajectory error using the high resolution NGM data is about 25% then the use of coarser resolution MRF data would result in absolute errors of about 42%.

HY-SPLIT verification during ANATEX was not just limited to trajectories and inert tracers. The meteorological database was used to test a sulfur wet deposition module (Rolph et al., 1992) that can be incorporated into HY-SPLIT. The particle emission routine was modified to permit simultaneous release of particles from each of the meteorological grid points with masses that corresponded to the sulfur dioxide emissions inventory for that grid square. The HY-SPLIT advection and dispersion algorithms easily handle multiple source emissions without any code modification. A dry and wet deposition routine that uses the NGM forecast precipitation and moisture was added and the model was used to predict 24 h air concentrations of sulfur dioxide and sulfate (SO_4^{2-}) wet deposition. In general, for a majority of the wet deposition monitoring

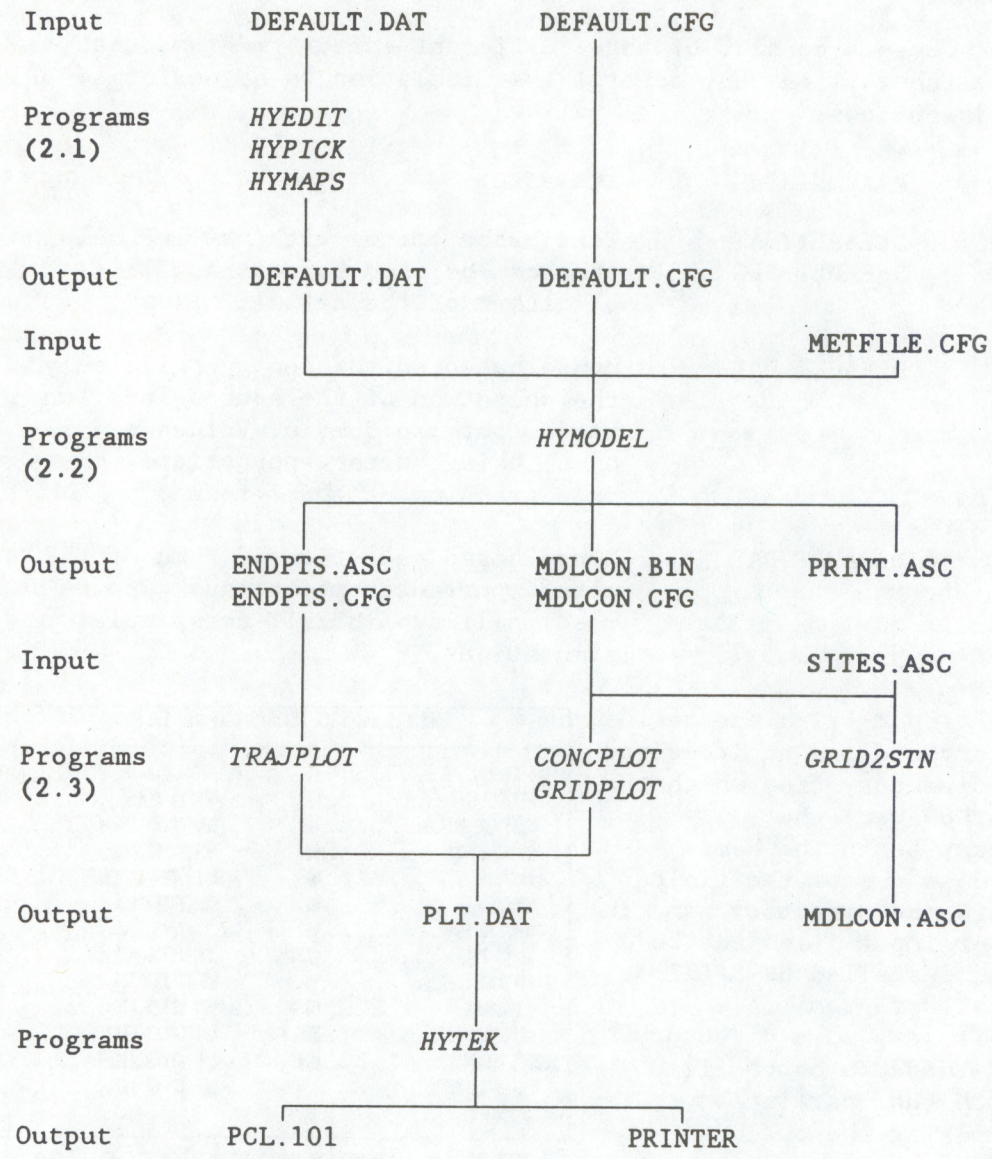
sites, the three month average model prediction to measurement ratios were between 0.5 and 1.6.

2. PROGRAM AND FILE STRUCTURE

Many of the technical details of the transport and dispersion calculations, and meteorological data are discussed in the Appendices, and will be noted as needed. However, any model consists not just of the primary calculational routines but many of the pre-processing requirements for the data as well as post-processing of the results for more meaningful interpretation. Obtaining correct results requires an understanding of the entire process, a modeling system, which may include many options and choices. One of the primary considerations of the main body of this report will be to link the different components so that the results do not just come from a "black box" but from a system that can be easily modified for different applications.

The modeling system is divided into three major components, a pre-processor for the input and meteorological data, the main transport and dispersion code, and a variety of post-processing graphics and support programs. The transport and dispersion model may require as many as five input files and may generate as many as six output files depending upon the options selected. Some output files are of course input files for other programs. The flow structure for the files used by the three major program elements and the program names are shown in Table 1. Not all input or output files are shown in this diagram, only the ones that are passed between program processes are illustrated. Program names are shown in italics. Other input and output files are discussed in Appendix G. The programs and files that correspond to each part of the HY-SPLIT model are discussed in the sections (2.1, 2.2, and 2.3) that follow.

Table 1.--Modeling system flowchart



2.1 Pre-processors

The ASCII files called DEFAULT.DAT and DEFAULT.CFG are the two primary files that contain much of the information that controls the model simulation. Most of the options that will be routinely changed are in the DEFAULT.DAT file (see Appendix E). Examples include such variables as the latitude and longitude of the source, meteorological data file names, and the type and frequency of output. Options that are changed less frequently are set in

DEFAULT.CFG (see Appendix F). Examples include such parameters as the coordinates of the meteorological and concentration sub-grids, and directories of input and output files.

The pre-processors consist of three different editor programs that can be used to modify input files that control the simulation to be performed. The features are as follows:

Code Name	File Edited	Features
HYEDIT	DEFAULT.DAT DEFAULT.CFG	Text based editor with on-line help that can be used to edit any line of either of the default files.
HYMAPS	DEFAULT.DAT	Mouse based editor that permits only the selection of the source location and output map domain. Values are set by clicking on the appropriate points on a graphics map background.
HYPICK	DEFAULT.DAT	Mouse based selection of some of the more important text options. Can be used in lieu of HYEDIT for simpler simulations.

In general input files can reside in any directory and are not required to be in the directory from which the model is run. However, the DEFAULT.CFG must be in the home directory because one of the fields in that file is the directory name in which all other input files can be found. If you installed HY-SPLIT with the install program (see Appendix G), it sets up a directory structure and loaded a batch file that works with that particular structure, invoking the options discussed in this section.

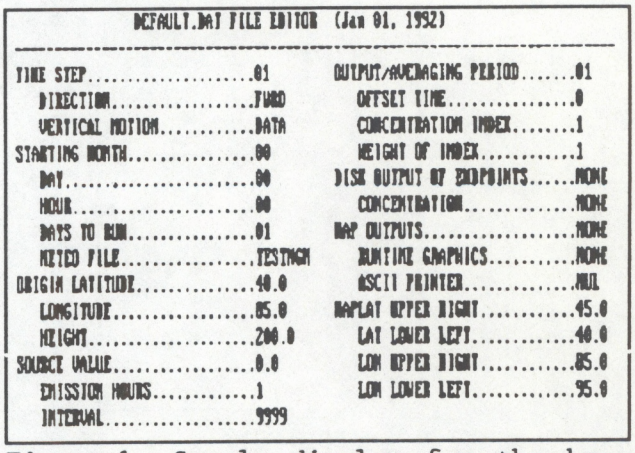


Figure 1. Sample display for the base case (test001) from the HYEDIT program.

The default files can be edited with any editor. The character text information after the # symbols in those files is only for convenience and is not required by the model. However, the text is used by the *HYEDIT* editor program. *HYEDIT* can be used to edit either the DEFAULT.DAT or DEFAULT.CFG files by invoking the DOS command line option of DAT or CFG (i.e. HYEDIT DAT or HYEDIT CFG). The advantage of using this editor is that it is customized for HY-SPLIT and help information is provided with each entry. An example of the display is shown in Fig. 1.

These settings shown in Fig. 1 will be used as the base conditions for all the following examples. The base case settings are also saved in the CFGFILE

sub-directory under the prefix TEST during the installation of HY-SPLIT. In all sections of this report, each example that will be discussed can be invoked through the batch file. For instance, the base case can be run by typing: HYSPLIT TEST001. Including the DAT option will bring up the menu shown in Fig. 1.

Individual entries are edited by using the cursor keys to place the marker over the desired entry. Pressing ENTER brings the entry to the edit line at the bottom of the display. When editing is complete press ENTER again to return to the main menu. ESC saves the changes and exits from the program. The help screen is invoked with CTRL-I. The help files HLPDAT.TXT and HLPCFG.TXT must be in the same directory as the *HYEDIT*. An expanded version of the help files is the main text of Appendices E and F.

Since the most frequently edited file is the DEFAULT.DAT file there are two additional editing options available if you have a mouse. It is necessary to first insure that the mouse is active by loading the appropriate software that came with the mouse. The program called *HYPICK* will bring up the display shown in Fig. 2.

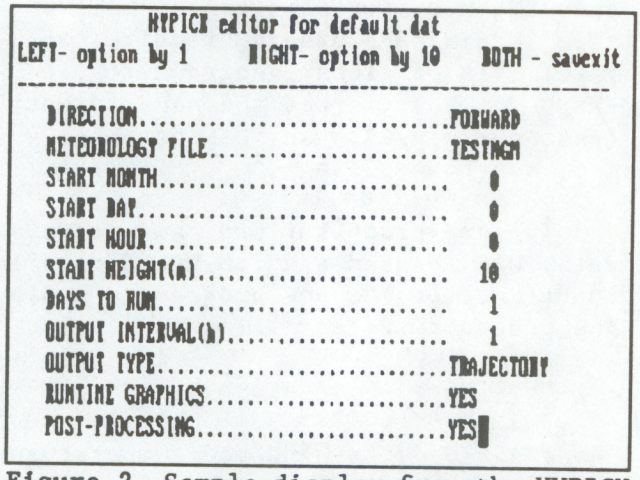


Figure 2. Sample display from the HYPICK default.dat mouse based file editor.

The program lets you select from a number of options by just clicking the left mouse button to scroll through the options by one or pressing the right button to increment the options by 10 each time. Pressing both left and right buttons saves the changes to the DAT file.

Only a limited number of the 27 input lines in DEFAULT.DAT can be edited with *HYPICK*. Selection of certain options automatically changes others within the file and certain options are set to default values each time the program is invoked. Some simulations require combinations of input parameters to be changed that are not available within *HYPICK*, therefore, *HYEDIT* must be used in those cases.

To set the source origin latitude, longitude and the latitude and longitudes corners of the output maps, you can use a program called *HYMAPS*. It draws a map background, as shown in Fig. 3, representing the meteorological domain of the file you selected for input in the DEFAULT.DAT file for the same example shown in Fig. 1.

The display shows a box representing the output map and red dot for the source location. You can then select a new map region by bringing the mouse to the lower left corner of a new map location, press the left mouse button and hold it as you move the mouse to the new upper right location, then release it and a new output domain box will be drawn. You can keep selecting new domains

until you get one you like. The map can be redrawn so that the sub-grid will fill the entire screen by clicking on the right button.

To select a new source location, press both buttons simultaneously and you will be in the source selection menu. At this point just move the mouse to the new source location, click the left button and the red dot will be redrawn. Press both buttons to continue on to the exit menu, where pressing the left button will save the new locations to the DAT file. The *HYMAPS* program requires an input file of global geography called EZMPDAT. The file has the same format (see Appendix G.3) as NCAR graphics map background files .

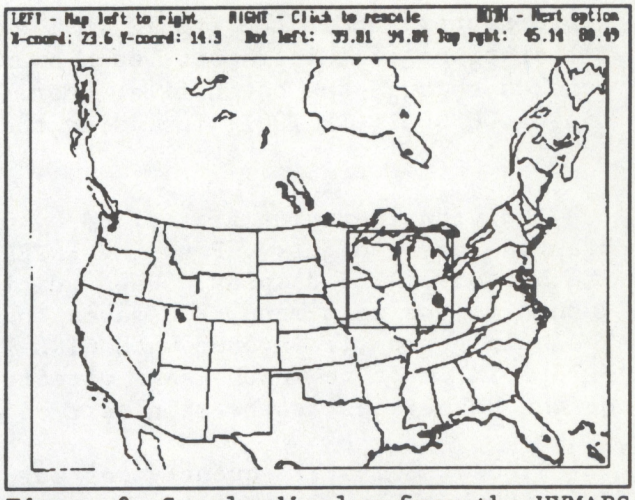


Figure 3. Sample display from the HYMAPS default.dat file mouse based editor program.

Two pre-processor programs are available to manipulate meteorological data. One to grid station-based data into a format compatible with the model input section and one program to manipulate the model compatible gridded data. The programs are as follows:

Code Name	Feature
WT2GRID	Wind and temperature soundings to gridded format
GAMDUP	General Archive Management Disk Utility Program

All meteorological data read by HY-SPLIT must be in the same packed gridded format. This format is described in detail in Appendix D. Although the format requirements are fairly strict, the type and number of variables, and order in the file are relatively flexible. HY-SPLIT contains an input data pre-processing section, within the main transport and dispersion module (*HYMODEL*) that converts the data or sets a variety of internal flags, to permit a more consistent set of calculations to be performed depending upon the available data and simulation options selected in the default input files. This data preprocessing is discussed in Appendix B.

The *WT2GRID* routines supplied with HY-SPLIT permit user supplied rawinsonde, surface, and pibal data, to be converted to the gridded input format consistent with Appendix D. This program is discussed in Appendix C. They are not designed to be as "user friendly" as other sections of the code due to large variations in input data formats. Most applications will require code changes and recompilation of the data input sections.

The utility routine, *GAMDUP*, is provided as means to manipulate the final gridded data. It is a self contained program that can be used to copy portions of a data file, extract sub-grids from a larger grid, check header

labels with each record, and perform other tasks. The details of that program, the options available, and the files required are discussed in section 3.4. In addition, several other programs (*GAMPOP* and *GAMGOP*) that can be used to unpack, print, and plot the meteorological data are discussed in that section.

2.2 Transport and Dispersion

The main transport and dispersion code is contained within the program *HYMODEL*. In addition to the two input files mentioned previously (DEFAULT.DAT, DEFAULT.CFG), four additional files are required. These are METFILE.CFG, ROUGLEN.BIN, EZMPDAT, and a scalable font file--MODERN.FON. Depending upon the options selected in DEFAULT.DAT, up to six output files may be generated.

The ASCII file METFILE.CFG contains information regarding the grid structure of various meteorological data files that the model may encounter. Before running with a new meteorological data source it is necessary to insure that the horizontal dimensions of the grid, its identification number, and scaling parameters are defined in this file. The data entry format for this file is given in Appendix G. Normally most data file structures are already defined in the file supplied with the program. If another data structure is created, the programs that are used to generate or extract the meteorological data will provide the necessary information for you to include in this file.

The model also uses the aerodynamic roughness length (ROUGLEN.BIN) to compute the vertical mixing coefficient for surface layer wind extrapolation. The data are given on a 1° lat/lon grid--the two byte binary format which is described in Appendix G--and upon input the model converts it to be compatible with the current meteorological data grid. This file is only required when the surface layer wind option is selected (See Appendix B, section 4).

If you select to compute run-time graphical output it is necessary to have the map background file: EZMPDAT. The same file is also used by a number of other programs: the *HYMAPS* editor and both *CONCPLOT*, *GRIDPLOT*, and *TRAJPLOT* post-processing graphics. The EZMPDAT file is in a format (Appendix G) compatible with NCAR graphics. Other compatible map background files can be substituted in its place. The EZMPDAT file contains global geography in about 500 kB, therefore, the resolution is limited to about 50 km. If you are running HY-SPLIT over a much smaller domain it is possible to obtain a replacement file for EZMPDAT that can have a maximum resolution of less than 1 km.

One last file not mentioned is the meteorological data. The file can have any name, although the default convention that is normally used is MONYR.BIN, where MON represents the month and YR the year. Therefore, data from April of 1990 would be placed in a file called APR90.BIN. The file name is set in DEFAULT.DAT. It is not necessary to include the BIN suffix unless the suffix is something else, then the full name is required. The directory for the meteorological data is set in DEFAULT.CFG.

The transport and dispersion calculations performed in the program called *HYMODEL*, is divided into nine components, each composed of several subroutines, that represent the major processes that must be modeled. If the optional Fortran source code is provided these are the file names that contain various subroutines. These elements include:

File Name	Description
MDRIVERS	Main program and other utilities
SETMODEL	Sets the conditions for the simulation
METINPUT	Inputs and processes the meteorology
EMISSION	Emits particles to represent the pollutant
TRNSPORT	Calculates the advection and dispersion
VPROFILE	Analyzes the meteorology at a grid point
SORTTING	Sorts the particles for greater efficiency
PLOTTING	ASCII based text plotting routines
GRAPHICS	Run-time screen based graphics displays

The normal ASCII screen display produced by *HYMODEL* during a simulation is shown in Fig. 4. The program identification is shown at start-up (from the batch file), then several diagnostic lines that describe the structure of the meteorological data file are printed. Then, if the data are properly read, the model positions to the starting record and the subsequent output is a simple digital clock printout each time step that shows the internal model time and the day-time field from the input meteorological data that apply for that model time step (in this case for the TEST001 example). In addition, the number of particles (or trajectories), the fraction of the released particle mass that is still on the computational grid, and the particle mass value that is used to determine which low-mass particles are dropped once per day, are shown at each computational time step.

```
      HY-SPLIT - Version 3.0 - April 1, 1992
   Hybrid Single Particle Lagrangian Trajectories
   Roland R. Draxler - NOAA/ARL (301) 713-0295

Press any key to continue . . .

Set meteorology grid:          6          33          28
Set meteorology file:          2           1           5
Positioned meteo rec:          0

MODEL TIME     DATA TIME      PARTICLES  RELEASE   CUTOFF
(MO DA HR)     (MO DA HR)     (NUMBER)   (FRAC)    (MASS)
 11  1  0      11  1  0           1       .00
 11  1  1      11  1  0           1       .00
 11  1  2      11  1  2           1       .00
 11  1  3      11  1  2           1       .00
 11  1  4      11  1  4           1       .00
 11  1  5      11  1  4           1       .00
 11  1  6      11  1  6           1       .00
 11  1  7      11  1  6           1       .00
 11  1  8      11  1  8           1       .00
 11  1  9      11  1  8           1       .00
```

Figure 4. Illustration of the ASCII screen display during a model simulation without run-time graphics (test001).

At the selected output interval, ASCII (without map backgrounds) concentration or trajectory maps can be displayed on the screen, printed, or saved to a file (PRINT.ASC) when that option is selected. If the run-time graphics mode is invoked the selected output will be drawn in real-time on the screen. All the run-time graphics examples will be shown in section 4. Normally error messages will appear on the screen, however, in run-time graphics mode, error messages will not appear on the screen, but will be written to a file called HYSPLIT.MSG. More detailed explanation of model error codes and their causes are given in Appendix I.

Individual particle or trajectory endpoints can be written to a file for post-processing graphics. Two files will be generated: ENDPTS.ASC with the actual endpoint data and ENDPTS.CFG with the map and labeling information required by the post-processing program. If concentration data are saved for post-processing two files are also created: MDLCON.BIN with the unformatted gridded binary concentration data and MDLCON.CFG containing the mapping and labeling information required by the mapping programs. Both file formats are discussed in more detail in Appendix G.

2.3 Post-Processing

In addition to run-time screen and printer output, one can set the model to output certain files that can be subsequently used by other programs to draw trajectory maps, concentration maps, or take the gridded concentration data and interpolate values at specific station locations. The graphics post-processing programs *CONCPLOT*, *GRIDPLOT*, and *TRAJPLOT* use NCAR graphics to generate a vector based graphics output file. This file can then be printed or displayed with the emulator program--*HYTEK*. The *GRID2STN* program is used to convert to output concentration values at specific locations on the grid--no graphics are involved. *HYVIEW* is used as an interface between calculated trajectories and the meteorological data by drawing soundings along the trajectory. The post-processing programs are as follows:

Program	Description
TRAJPLOT	Draws a trajectory from endpoint positions
CONCPLOT	Draws a density weighted concentration image
GRIDPLOT	Prints the concentrations at each grid point
GRID2STN	Interpolates the gridded concentrations to a point
HYVIEW	Display Skew-T diagrams along a given trajectory
HYTEK	Interprets a Tektronix 4010 file

If the post-processor graphics option is chosen, the plotting programs read their respective input files and generate a graphics output file called PLT.DAT. No input prompts are available with the first three graphics programs. The *HYMODEL* code generates the control files ENDPTS.CFG and

MDLCON.CFG. These can be edited prior to running the graphics programs if other output options are desired. The format for these files is discussed in Appendix G.

When the vector graphics output file PLT.DAT is generated one may either display it, print it, or both. Since it is in standard Tektronix 4010 format, any commercial emulator can be used. For convenience a simple emulator, *HYTEK*, is supplied with HY-SPLIT. It can be used to display or print the graphics on a dot matrix, laser jet, or paint jet printer. Detailed operating instructions for *HYTEK* are given in Appendix H.

The program *GRID2STN* can be used to read the MDLCON.BIN file and interpolate the concentration data to specific latitude and longitude sites. The program reads a file called SITES.ASC with the station names and positions and generates an ASCII output file with the corresponding concentrations at each station. The first record in SITES.ASC contains the conversion factor applied to all gridded concentration data. This is used to generate integer rather than fractional output values. Formats for these files are also described in Appendix G.

HYVIEW is a mouse driven screen display program that can be used to point to a location and time on the calculated trajectory map and the plot the wind, temperature, and dew-point profiles in a Skew-T format. It can use the same meteorological data that was used to calculate the trajectory. You will be prompted to enter the meteorological data file name. The trajectory position at each output step is displayed on the display map background. Clicking on the right mouse button increments the time along the trajectory highlighting a different end-point position. The spatial location of the mouse pointer designates the meteorological grid location. Clicking on the left mouse button will display a Skew-T sounding at that location and time. If the pointer is over the trajectory the sounding at that location will be displayed. Pressing both buttons simultaneously exits the program. No hard-copy option is provided beyond the conventional DOS screen dump.

3. METEOROLOGICAL DATA

Spatial and temporal density of the input meteorology is probably one of the most important factors controlling advection and dispersion calculations. The HY-SPLIT code was designed to use previously gridded data in synoptic (time series) format. There are two options: (1) data are available only at rawinsonde and surface observation points or (2) data have already been gridded. Regardless of the source, the gridded data are assumed to be in a format as described in Appendix D before being read by the model. For option 1, a pre-processor program is available to grid the data as required (see Appendix C). For option 2, the gridded data have already been archived in the proper format. The meteorological data then read by *HYMODEL* are first processed (see Appendix B) to compute the necessary diagnostic variables required in the model calculation. These calculations depend in part upon what

variables are in the data set and what run-time options have been selected. The primary diagnostic variables computed for dispersion and advection calculations are the vertical velocity (if not available from the input data) and the vertical mixing coefficient profiles at each grid point over the model domain.

3.1 Upper Air and surface observations

A program called *WT2GRID* is provided to convert twice-daily rawinsonde and surface observations to the standard HY-SPLIT gridded format. The program assumes that the rawinsonde data are in NAMER-WINDTEMP format. At each synoptic time all the wind observations come first followed by all the temperature soundings. The appropriate subroutine (INPNMR) within the *WT2GRID* code can easily be modified to accept data in other formats. The twice-daily soundings are linearly interpolated to any desired temporal frequency. If they are available more frequently at some stations, these observations replace the interpolated values at grid points adjacent to the stations.

WT2GRID also accepts more frequent (usually 3 hourly) surface observations in a format similar to NCDC's TD-1440 (airways surface observations). Other input data formats can be customized in the INPSFC subroutine. The optional surface observations are used in two ways. First, they replace the lowest level wind observations at all primary and interpolated rawinsonde observation times (assuming a 3 h interpolation interval). Second, the surface temperatures at the grid points replace the interpolated sounding temperatures at the lowest level. The new surface temperature in conjunction with the lowest level interpolated sounding temperature will then be used to compute a vertical stability (and subsequent mixing coefficients) that more accurately reflect the diurnal cycle.

Once configured for a particular input data configuration and format the program requires four entry lines: the starting and ending dates, and the input and output file names.

WT2GRID

```
Start  (inclusive): YR MO DA
Ending (exclusive): YR MO DA
Input rawinsondes file:
Output binary file:
```

Rawinsonde data in a format that *WT2GRID* has been configured to accept is available from the National Climatic Data Center (NCDC), Asheville, North Carolina 28801. Each NCDC tape contains six months of rawinsonde data for North America. The tapes are called NAMER-WINDTEMP and are archived under the tape deck identification number TD-9743.

3.2 NMC gridded archive and forecast data

The primary sources of gridded archival data are from the National Meteorological Center's (NMC) Nested Grid Model (NGM) and from the final analysis of the Medium Range Forecast model (MRF). The HY-SPLIT gridded data format is somewhat different from that used by NMC. The NMC data are read, converted, and archived by ARL for transport and dispersion modeling purposes. The format differs primarily to conserve space and to maintain a fixed record length to make it possible to randomly position the record pointers of the model within a large data file.

The primary source for archival data over the continental U.S. is from NMC's Nested Grid Model (Phillips, 1975). The archive data consists of a series of 12 h forecasts made twice a day to generate a long time series of diagnostic model data. Although the NGM computational grid is 90 km and it is available every hour for the first 12 h, to conserve space only every other grid point and every other hour is saved for the archive. This achieves a considerable space savings with a minor loss of trajectory accuracy. Data are available from January 1989 and consistently (from NCDC) after January 1991. Vertical resolution in the terrain following sigma coordinate system is quite good with 10 levels available between the surface and about 400 mb.

In addition to the archive data, the hourly 90 km computational data are available in real-time on our in-house computer system. They are, however, overwritten each day. Upon sufficient notice it is possible to save these data for special applications.

Operationally we also obtain the NGM forecast out to 48 h after the initialization. These data are output only every 6 h on a grid which has a resolution of about 180 km. These forecasts are also overwritten each day and are not saved.

Global coverage is obtained by saving analyses from NMC's Global Data Assimilation System (Kanamitsu, 1989; Derber et al., 1991). The analyses are produced by combining observations with 6 h Medium Range Forecast model forecasts and are available at the four primary synoptic times (0, 6, 12, and 18 UTC). The output is converted to ARL format on a 381 km polar stereographic grid for each hemisphere. The data archive consists of the northern hemisphere data followed by the southern hemisphere data for each synoptic time. These data have only been archived since January 1991.

Similar to the NGM, the MRF forecasts to 72 h are downloaded twice-daily to the ARL computer and are available for computational use. They are however, overwritten with each forecast. Usually only the northern hemisphere forecasts are available. Southern hemisphere forecasts can be initiated upon request. One limitation of the MRF data with regard to boundary layer research, is that it is routinely available only on mandatory pressure surfaces.

Gridded meteorological model output data archived from the NGM and MRF in a format that HY-SPLIT is configured to accept is available from the National Climatic Data Center (NCDC), Asheville, North Carolina 28801. Each NCDC tape

contains six months of NGM data (North America) and two months of MRF data (both northern and southern hemispheres). The tapes are archived under the identification number TD-6140.

3.3 Special Observational Data

A variety of special application output options are available by special request to ARL. These can be initiated for special experiments or in response to major accidents that result in the atmospheric release of substances that can affect human health. In particular, one option permits re-computation of the gridded output directly from the spectral coefficients of the MRF, so that a high resolution (90 km) output window can be set up anywhere on the globe. This is a rather computationally prohibitive program and is not available for routine use.

3.4 Data archive management

There are three programs in this group all starting with the GAM acronym--General Archive Management. There is the Disk Utility Program (*GAMDUP*) to manipulate the archived meteorological data; the Printer Output Program (*GAMPOP*) to print the horizontal field for an archive variable or the sounding for all variables at a specific location; and the Graphics Output Program (*GAMGOP*) which can be used to contour the data fields over a map background.

These programs are installed to the UTILITY sub-directory and use METFILE.CFG for input. The data must reside on a PC disk file and you will be prompted to enter the complete file name (directory\name) within single quotes. The *GAMGOP* program generates a PLT.DAT file as output and you can use *HYTEK* to view that file. A sample menu for each program is shown below; however, each specific option requires additional input information.

GAMDUP

```
Input meteorological file (within single quotes):

SELECT OPERATION
0 - exit
1 - check headers
2 - inventory OR fill missing
3 - first and last group
4 - data copy by record
5 - data copy by day
6 - sub-grid data extraction

? - PLEASE SELECT NUMBER
```

The first entry is the meteorological data file name. The subsequent entry is the number of the operation that will be performed on the file. At this time six options are available:

1 - "Check headers" displays the ASCII header label at the beginning of each meteorological data record. These can show every record or just one observation time each.

2 - "Inventory or fill missing" checks for gaps or duplicate data in the file and list those affected records. Options include creating a new file without the problems. Under normal situations the HY-SPLIT code will properly pass through missing data and there is no need for a fix.

3 - "First and last group" examines the first and last time group on the file given an input of how many days of data are required to be on that file. It is a quick way to check a file for the proper number of records.

4 - "Data copy by record" permits extraction of specific records from the file to be copied to another file.

5 - "Data copy by day" permits extraction of a specific number of days from a particular start day to be copied to another file.

6 - "Sub-grid data extraction" is the extraction of a sub-grid from the full grid in the input file. The extraction can be done as a data copy "by day" or for the entire file. The extraction option takes a little time as the data must be unpacked and repacked in the new grid. The new grid must be defined in METFILE.CFG before the extraction option is attempted.

The *GAMDUP* routines are continually subject to modification. Care should be exercised when using *GAMDUP* as it is possible to modify your data in such a way that it cannot be used by HY-SPLIT.

The Printer Output Program only has two menu choices at this time. One for printing a sounding at a specific latitude and longitude (it uses data from the nearest grid point) and an option to print out the numeric data in an ASCII integer format at a particular level (MAP option). The sample input menu is shown below.

GAMPOP

```
Input meteorological file (within single quotes):

SELECT OPERATION:
0 - EXIT
1 - SOUNDING
2 - MAP

? - PLEASE SELECT NUMBER
```

After starting an option you will be prompted for other inputs. Please see the *GAMGOP* discussion below as the requirements are very similar.

The Graphics Output Program is used to generate graphics output, however, at this time there is only one active option: the contoured map, cross-sections are not yet available. The input menu, shown below, is similar to the previous ones.

GAMGOP

```
Input meteorological file (within single quotes):

SELECT GRAPHICS OPERATION
0 - exit
1 - contoured map
2 - cross-section

? - PLEASE SELECT NUMBER
```

Upon starting the map option you will be prompted for several inputs such as the latitude and longitude of the display map corners, aspect ratio, and several other parameters. These are all assigned default values and it is only necessary to enter the line feed character (/) followed by the ENTER key to accept the defaults. This is the recommended procedure unless you are not satisfied with the default map display. After the first set of inputs a table will be displayed showing all the potential variables in the meteorological data file by their 4 character code. Most identifications are obvious, for others refer to Appendix D. At this stage it is only necessary to select the time (day and hour) and the variable number and sigma level. Note that surface level variables are identified by level 0. The tabular options menu will be displayed after each frame is completed. You may generate as many frames as you like in the output file PLT.DAT before using *HYTEK* to print or display each frame.

4. HY-SPLIT OUTPUT OPTIONS

The HY-SPLIT model calculation results can be displayed on the screen or printer while the model is running. Options can be set in the DEFAULT.DAT file to create certain output files so that post-processing graphics programs can be used to display particle positions, trajectories, or maps of air concentrations on a variety of graphics devices. In this section examples of the various output options will be shown and explained.

As noted earlier, all examples are given in the CFGFILE directory under the file names TEST00?.DAT and .CFG. Upon invoking the HYSPLIT batch file, for example with the DOS command line: HYSPLIT TEST003, the TEST003 files will be copied to DEFAULT.DAT and DEFAULT.CFG. The DEFAULT files are used by the

editors and then by the model to control the simulation. Changes made to the base case by line number will be given with each example. Except when noted otherwise, these line numbers refer to the lines in the DEFAULT.DAT file as summarized in Appendix E.

The following examples can be used to develop your customized DEFAULT files. After modifying and editing a standard TEST case with your own configuration options, run the model to confirm the results and then rename the DEFAULT files in the CFGFILE sub-directory to some other name. Subsequently you may then invoke that name on the command line when you run the HYSPLIT batch file.

4.1 Run-time Displays

One of the simpler displays is the particle position map, or snapshot. This map illustrated in Fig. 5 shows the position of all the computational particles at a particular instant--Nov 01 at 2300 UTC. The date and time in the upper left corner of the sample gives the time of the snapshot. The first three lines are the same as the ASCII screen display, except they are overwritten each time step.

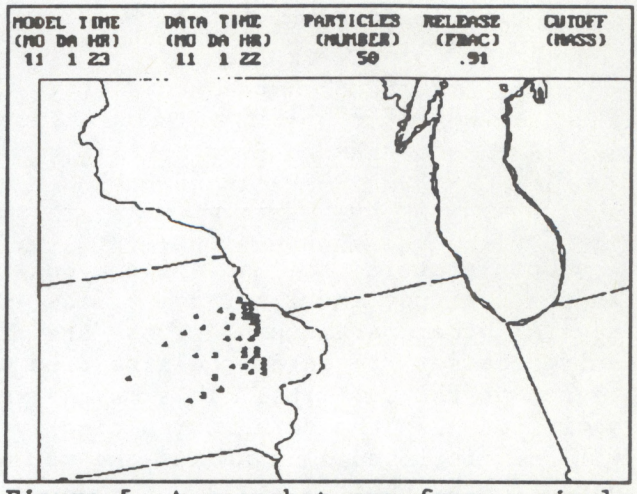


Figure 5. A snapshot map from a single release (test002) after 24h travel.

This simulation is given in TEST002. Only three lines were modified from the base case file (TEST001): the source term (line 12) was changed from 0.0 to 1.0, the map output type (line 21) was set to SNAP, and the run-time graphics option (line 22) was set to YES. The projection is polar stereographic and the display window latitude/longitude coordinates are set in the DEFAULT.DAT file. The origin location is indicated by the asterisk and the position of each particle is represented by a number indicating the maximum meteorological data level reached by any particle in that print position.

In this illustration the source was only a single particle released 24 h ago at 0000 UTC near the Indiana/Ohio border. The illustration in the figure is only at one time. If you were running this case on the computer you would see the display updated each time step, as the particle moves to a new position. These kinds of displays are useful for positioning aircraft or similar real-time requirements. Another application of the snapshot display is that when it is updated every time step, running on a sufficiently fast computer, the resulting display becomes an animation of the pollutant position with time.

A trajectory example is shown in Fig. 6. This display shows the path a single particle would have taken had it been released at the start time indicated in the DEFAULT.DAT file. Note that in the base case (Fig. 1) no

start time is indicated. This means that the model will use the first observation in the meteorological data file as the start time for all calculations. The release height for this case, as all others, was set to 200 m, about the first sigma level of the NGM. The simulation is given in the TEST003 file and only two changes were made from the last example: the source term (line 12) was set back to 0.0 and the display output (line 21) was set to TRAJ.

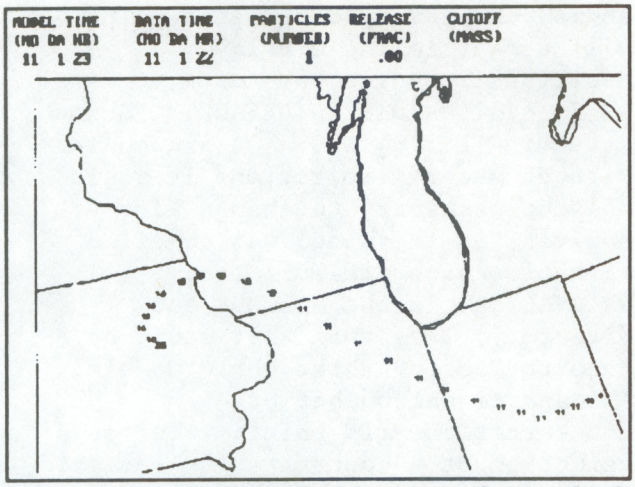


Figure 6. Trajectory map after 24-h travel time with positions shown hourly (test003).

The TRAJ display is similar to the snapshot, except that the particle positions as a function of time are indicated by a two digit number. The first digit is the travel time day with respect to the release day (1-first day, 2-second day, etc.) and the second digit is the sigma level. Note that the meteorological data level starts at 1 and increases with time to 5 due to the vertical motion associated with the low pressure system.

If you were watching this example in real-time the display would be updated each time step with an additional position. The old positions, as opposed to a snapshot display, would not be erased. In Fig. 5 the old display is erased before each new output. The particle position is shown each time step (line 1). However, if you do not want to see the display updated each time step you can set line 15 to some other output interval, perhaps the end of the trajectory, 24 h.

An example of the average grid point concentrations for the same 24 h period as in the preceding example is shown in Fig. 7 and given in the file TEST004. The only changes made to the previous example was that the source (line 12) was set back to 1.0, the output period (line 15) was set to 24, and the output type (line 21) was set to CONC. The height at which the concentrations apply was set in the base case to 1 meter.

Concentrations are represented by three digits; the central digit is located over the grid point. The first digit is the mantissa, the second and third is the negative exponent. For example, near the source point the 713 would be interpreted as a concentration of 7×10^{-13} mass units per cubic meter. Notice the regions of concentration are larger than the corresponding particle positions because the concentrations are 24 h averages representing contributions to each grid point that has been intercepted by the particle trajectory.

In this example an additional change was made to the DEFAULT.CFG file to permit concentration to be output at a grid interval of 90 km rather than the 180 km meteorological grid. If you only make changes to the file as indicated

above, only every other grid point will appear in the display. Additional changes were made to lines 1, 2, 6, 7, and 9 in DEFAULT.CFG and saved in TEST004.CFG. On a computer without memory limitations it would only be necessary to change line 9; however, as the model was compiled with dimension maximums (see GRIDVAL.DAT in the MDLCODE sub-directory) less than what would be required to cover the whole domain. The additional number of concentration grid points requires a selection of a concentration sub-grid (lines 1, 2, 6, and 7). If you forget to make these changes the concentration grid will default to the lower left corner of the meteorological grid and the display may not show any concentrations over the selected display region.

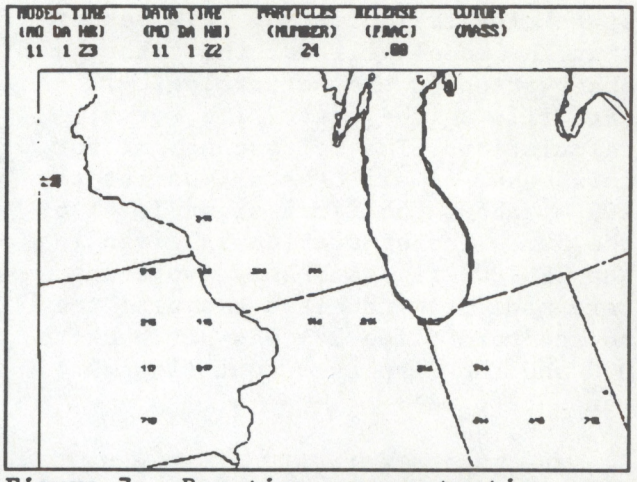


Figure 7. Run-time concentration map display (test004) showing the 24-h average values.

4.2 Post-processing Displays

Post-processing graphics is controlled by a batch file, PLOTTER, in the GRAPHIC sub-directory. It is called by the main batch file, HYSPLIT. The various programs described below are called if the main program, as controlled by the input parameters, produced the correct output files required as input to these programs.

The two types of displays that can be created after the model is run are similar to the run-time options. The trajectory case, shown in Fig. 8 (TEST005), is the same case as illustrated in Fig. 6. The only change to the base case file was that the endpoints to disk option (line 19) was set to STEP. Now the trajectory is shown by a smooth solid line, with hash marks every 6 h. At the bottom of the map is a projection of the trajectory in the vertical plane for the corresponding horizontal positions. The ordinate for the vertical projection is millibars. Note the upward movement of the trajectory as it approaches the low pressure system. The label at the top of the map is the trajectory starting time. The TRAJPLOT program reads the trajectory output

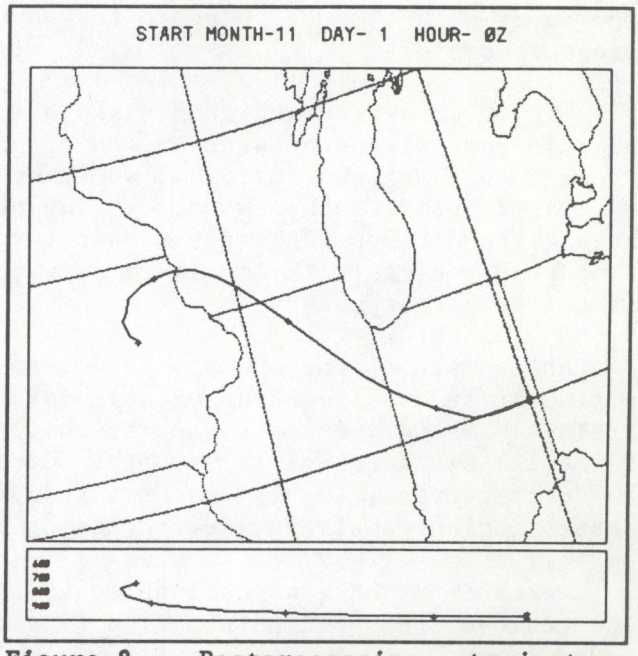


Figure 8. Postprocessing trajectory output from TRAJPLOT (test005) is identical to that shown in Fig. 6.

file ENDPTS.ASC and creates a graphics file called PLT.DAT. The illustration shown in Fig. 8 is obtained by displaying that file with a program called HYTEK (see Appendix H).

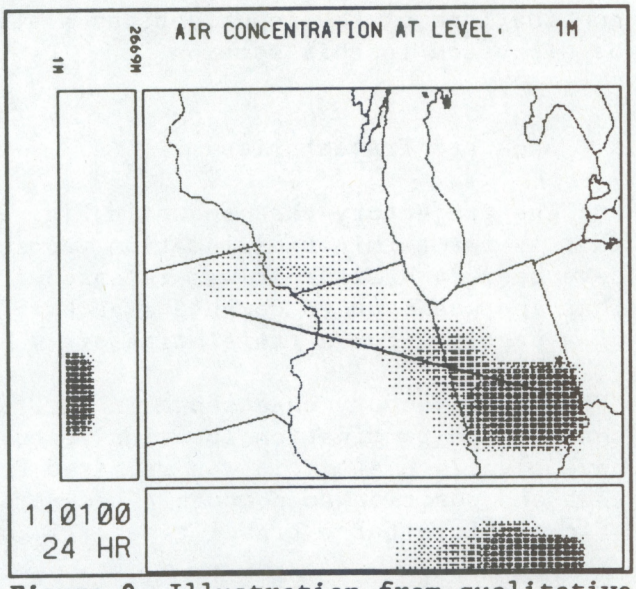


Figure 9. Illustration from qualitative concentration display (test006).

High-resolution qualitative concentration graphics output is generated by a program called *CONCPLOT*. The display is shown in Fig. 9 (TEST006). This is the same simulation as shown in Fig. 7 with only a change to the concentration to disk parameter (line 20) of WRITE. The time (month 11, day 01, and hour 00) at which the concentration average is started is indicated in the lower left corner above the averaging period in hours. The large central panel shows the same concentration field as in Fig. 7 with the dot shading density corresponding to the magnitude of the concentrations. The lower and left side panels show the vertical concentration profiles in the east-west (bottom) and north-south (left) grid directions, respectively, along the straight line in the central panel that is the most parallel to the projection direction. The north-south line in the central panel is obscured. The heights along the sidebars indicate the minimum and maximum vertical domain in meters of the concentration grid.

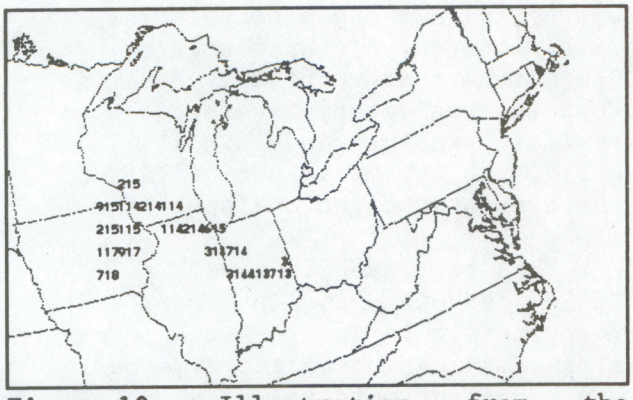


Figure 10. Illustration from the quantitative concentration display.

Quantitative concentration maps, similar to the display shown in Fig. 7, is created by the special program *GRIDPLOT*. The same simulation setup as in TEST006 is used for this example shown in Fig. 10. The concentrations are interpreted the same way as in Fig. 7. The setup that produces the qualitative concentration map creates the MDLCON.BIN output file, which is also used by the *GRIDPLOT* program. The only difference is that *GRIDPLOT* must be called by its own program name, as the HYSPLIT batch file is designed to call the *CONCPLOT* program when a MDLCON.BIN file exists. This can of course be changed to suit individual needs. The main difference between this display and the one generated during the model run is that the *GRIDPLOT* display will always show the entire concentration grid domain, regardless of the display map domain selected in the DEFAULT.DAT file.

5. SPECIAL EXAMPLES

There are many different simulations that can be performed by various combinations of the input options available. Several additional examples will be discussed in this section.

5.1 Backward Trajectories

The trajectory case shown in Fig. 6 was calculated in a forward direction, that is the termination location represented the position a particle would have been 24 h after it was released from the origin position. We can take that end position to compute a backward trajectory which will show the origin of a particle for a travel time of 24 h upwind.

The trajectory case shown in Fig. 6 was calculated in a forward direction, that is the termination location represented the position a particle would have been 24 h after it was released from the origin position. We can take that end position to compute a backward trajectory which will show the origin of a particle for a travel time of 24 h upwind.

The changes required to the default file are that the direction (line 2) is set to BACK, and the starting time must be explicitly stated (lines 4, 5, and 6) as month 11, day 01, and hour 24. The starting time must be set to day-1 hour-24 rather than day-2 hour-0 because the model is unable to position to the end of the one-day meteorological data file (day-2 does not exist). One unique feature of this case is that the trajectory is started at a specific pressure level in millibars designated by the letter "P" after the pressure height on input line 11.

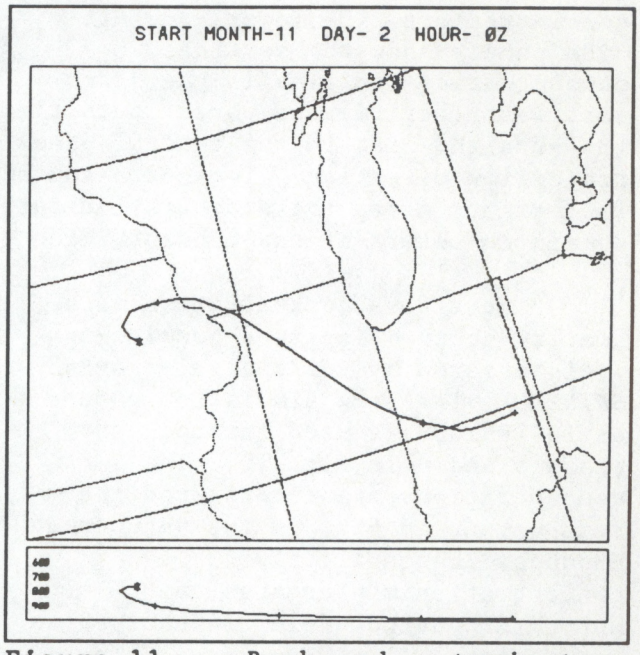


Figure 11. Backward trajectory computation (test007) for the forward case shown in Fig. 6.

This test case is saved in TEST007 and is shown in Fig. 11. Now when the simulation runs the model starts at the end of the time period and reads the meteorological data file backwards in time calculating the trajectory advection with a negative time step. The backward trajectory is only a little south and west of the initial starting location. This small difference represents the numerical errors associated with the trajectory computation. This example would be typical of some of the largest numerical errors due to the extreme curvature and vertical motions at the trajectory start in the vicinity of the low pressure system.

5.2 Vertical Motion

In all the previous simulations the vertical motion option, line 3, was set to DATA. The calculation used the omega term output by the NGM. If that is changed to computing the divergence, DIVG (TEST008), the resulting trajectory is shown in Fig. 12. This is the same case as shown in Fig. 6 with the exception that now the vertical velocities are computed internally within HY-SPLIT from the divergence of the horizontal velocity field. The velocities tend to be smaller and the resulting trajectory stays closer to the first sigma level.

This illustrates that horizontal trajectories can be very sensitive to the vertical velocity option. This is of interest because some meteorological data sources do not report vertical velocities and hence they must be estimated by other means.

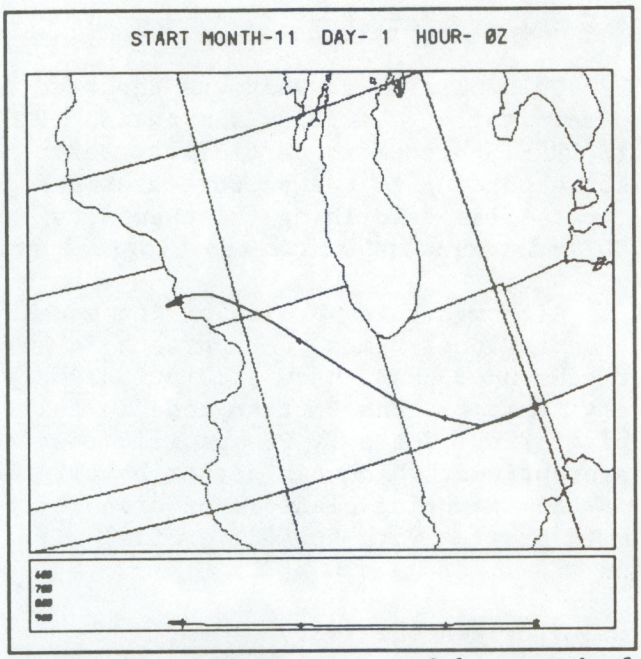


Figure 12. Trajectory with vertical velocity computed from the divergence field (test008).

6. MISCELLANEOUS APPLICATIONS

One major advantage of the HY-SPLIT code structure is that usually only one or two subroutines need to be modified to change the nature of the modeling simulation. Each option discussed in this section requires a version of HY-SPLIT that has been compiled with the changes noted in each subsection.

6.1 Multiple Source Emissions

Repeated emissions at regular intervals at the same location can be handled through the normal setup procedure in the input file DEFAULT.DAT. When simultaneous emissions at multiple source locations are desired it is only necessary to make a few changes to the main program that calls the SOURCE subroutine. A table of source locations and loop that calls the SOURCE subroutine for each emission location must be added to the main program. All internal arrays, trajectory, and concentration calculations automatically account for the multiple particle positions that are generated. Trajectory display outputs may however become difficult if not impossible to read.

6.2 Sulfur Chemistry

This version is what was reported by Rolph et al. (1992) and requires a precipitation chemistry subroutine (PRCHEM), a new emissions subroutine (SOURCE) that emits particles at each meteorological grid location corresponding to the sulfur emissions in that grid square, and various other input files describing the chemistry rate constants, and the seasonal SO_2 and SO_4 emissions in each meteorological grid square.

Although this version of the model can be run on a DOS based PC, computational times can approach 24 h for a seasonal simulation. It is recommended that these simulations be performed in a UNIX based workstation environment. The Fortran code is fully compatible with other computing platforms. The only PC specific routines are the run-time graphics subroutines, which can either be altered to reflect the graphics environment of the computing platform or disabled by commenting out all subroutines in the main program with the GRF prefix.

6.3 Nitrogen Chemistry

The nitrogen chemistry option is similar to that of sulfur in that it includes the sulfur as well as the nitrogen chemistry. A formal report describing the testing of this option is not yet available. The coding and structure follows that of sulfur. However, due to the additional chemical species that must be carried along in the computation it is not possible to run this version on a DOS based PC.

6.4 Particles, Deposition, and Decay

A generic dry and wet deposition subroutine with gravitational settling and radioactive decay may be included in the subroutine library. These calculations are only performed if the deposition configuration file (DEPVEL.CFG) is included in the input files sub-directory. Otherwise no mass depletion occurs. Required parameters in this file include particle density, size, molecular weight, reactivity constants, half-life, leaf-area-index, and several other hard to determine parameters.

6.5 Radiological Routines

Specific radiological dose calculations are only performed in the post-processing environment. However during the transport and dispersion calculations, the model does calculate the effects of radioactive decay and those results are saved to the gridded concentration output file. This file, which includes deposition amounts as well as air concentration is then read to produce dose estimates. This routine is under development and will only be available for a limited number of species.

7. ACKNOWLEDGMENTS

This research was sponsored by the U.S. Air Force Technical Applications Center.

8. REFERENCES

Businger, J.A., 1973: Turbulent transfer in the atmospheric surface layer. Workshop on Micrometeorology, August 14-18, 1972, D.A. Haugen (Ed.), American Meteorological Society, Boston, 67-100.

Byers, H.R., 1974: General Meteorology. McGraw-Hill, New York, 461 pp.

Clark, T.L. and Cohn R.D., 1990: The Across North America Tracer Experiment (ANATEX) Model Evaluation Study, EPA/600/3-90/051, June, U.S. Environmental Protection Agency, Research Triangle Park, N.C.

Danielson, E.F., 1961: Trajectories: Isobaric, isentropic, and actual. J. Meteorol. 18:470-486.

Derber, J.C., D.F. Parrish, and J.J. Lord, 1991: The new global operational analysis system at the National Meteorological Center, Weather and Forecasting 6:538-547.

Draxler, R., 1982: Measuring and modeling the transport and dispersion of Kr-85 1500 km from a point source. Atmos. Environ. 16:2763-2776.

_____, 1986: Simulated and observed influence of the nocturnal urban heat island on the local wind field. J. Clim. Appl. Meteorol. 25:1126-1137.

_____, 1987: Sensitivity of a trajectory model to the spatial and temporal resolution of the meteorological data during CAPTEX. J. Clim. Appl. Meteorol. 26:1577-1588.

_____, 1990: The calculation of low-level winds from the archived data of a regional primitive equation forecast model, J. Appl. Meteorol. 29:240-248.

_____, 1991: The accuracy of trajectories during ANATEX calculated using dynamic model analyses versus rawinsonde observations, J. Appl. Meteorol. 30:1446-1467.

_____, and A.D. Taylor, 1982: Horizontal dispersion parameters for long-range transport modeling. J. Appl. Meteorol. 21:367-372.

_____, and B.J.B. Stunder, 1988: Modeling the CAPTEX vertical tracer concentration profiles. J. Appl. Meteorol. 27:617-625.

_____, R. Dietz, R.J. Lagomarsino, and G. Start, 1991: Across North America Tracer Experiment (ANATEX): Sampling and Analysis, Atm. Environ. 25(A):2815-2836.

Heffter, J.L., 1965: The variation of horizontal diffusion parameters with time for travel periods of one hour or longer. J. Appl. Meteorol. 4:153-156.

_____, 1980: Transport layer depth calculations. Second Joint Conf. on Applications of Air Pollution Meteorology, March 24-27, 1980, New Orleans. American Meteorological Society, Boston, 787-791.

Hunt, J.C.R., 1985: Diffusion in the stably stratified atmospheric boundary layer. J. Clim. Appl. Meteorol. 24:1187-1195.

Kanamitsu, M., 1989: Description of the NMC Global Data Assimilation and Forecast System, Weather and Forecasting 4:335-342.

Lange, R., 1978: ADPIC--A three dimensional particle-in-cell model for the dispersal of atmospheric pollutants and its comparison to regional tracer studies. J. Appl. Meteorol. 17:320-329.

O'Brien, J.J., 1970: A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer. J. Atmos. Sci. 27:1213-1215.

Phillips, N.A., 1975: The Nested Grid Model. NOAA Tech. Rep. NWS-22, U.S. Department of Commerce, Silver Spring, MD, 80 pp.

_____, 1986: Turbulent mixing near the ground for the Nested Grid Model. Office Note 318, National Meteorological Center, National Weather Service, Silver Spring, MD, 19 pp.

Pielke, R.A., and Y. Mahrer, 1975: Representation of the heated planetary boundary layer in mesoscale models with coarse vertical resolution. J. Atmos. Sci. 32:2288-2308.

Rolph, G.D., and R.R. Draxler, 1990: Sensitivity of three-dimensional trajectories to the spatial and temporal densities of the wind field, J. Appl. Meteorol. 29:1043-1054.

Rolph, G.D., R.R. Draxler, and R.G. de Pena, 1992: Modeling sulfur concentrations and depositions in the United States during ANATEX, Atm. Environ. 26(A):73-93.

Van Ulden, A.P., and A.A.M. Holtslag, 1985: Estimation of atmospheric boundary layer parameters for diffusion applications J. Clim. Appl. Meteorol. 24:1196-1207.

APPENDIX A - TRANSPORT AND DISPERSION

The model can be run in two basic modes: transport alone or transport with dispersion. If only the transport option is selected, then each particle that is released will be advected and its position calculated each time step without any horizontal or vertical dispersion. One can equate this to following the pollutant centroid position, and it is represented by a single latitude and longitude. The transport only option is available either in forward or backward modes. In a backward mode the advection time step is negative, meteorological data are read sequentially backward in time from the starting time, and the resultant trajectory represents the upwind source of material at the specified starting location and time.

The transport and dispersion option permits each released particle to disperse and potentially divide into many more particles to represent the pollutant distribution. This option should not be confused with the trajectory option above. If trajectory output is selected with the dispersion option, a complex pattern may result due to the many particles that can be generated by a single release due to particle division. The transport and dispersion option is not available in the backward mode because atmospheric dispersion is not a reversible process. Essentially when a backward trajectory is started at a receptor one does not know if or how much of the pollutant is mixed toward the receptor from above or below. The only way to properly attribute emissions through a hybrid-receptor modeling approach, without the use of "diffusing" backward trajectory calculations, is to run a model from each of the potential source regions to calculate concentrations at the desired receptor and then through statistical methods apportion the emissions.

A.1 Trajectory and Advection Computations

Each particle is identified by its mass Q, horizontal position in cartesian grid coordinates by the horizontal position vector X, pressure P, and horizontal σ_h and vertical σ_v standard deviations of its position. The horizontal advection of the particle from the initial position X_0 to the final position X_2 over the time step Δt (line 1 in DEFAULT.DAT) is computed by

$$X_2 = X_0 + 0.5(V_0 + V_1)\ \Delta t\ , \qquad (1)$$

where V_0 is the horizontal wind vector at the initial position X_0 and V_1 is the wind at position

$$X_0 + V_0\ \Delta t\ . \qquad (2)$$

This method is a simple first-order approximation to account for curvature in the wind field. The final horizontal position is computed as the distance weighted average of X_2 computed using winds at the nearest data levels below and above the initial particle height P_0 (line 11 in DEFAULT.DAT).

The new vertical position or pressure of the particle is given by

$$P_2 = P_0 + 0.5(W_0 + W_1)\ \Delta t \ . \qquad (3)$$

The vertical velocity W_1 (total derivative of pressure) is defined at the same position as V_1. A linear interpolation from the data grid is used to define meteorological variables at the particle position. Particles can exit the model top or will run along the model terrain surface as defined by the surface pressure field. Other options (line 3 in DEFAULT.DAT) include: isobaric calculations, where W = 0; and an isosigma calculation, where the particle maintains a constant ratio of P/P_{sfc}. In addition, if the vertical velocity field is not available in the input meteorological data field, the vertical velocity can be defined by integrating the velocity divergence

$$W = -\int^z (\partial u/\partial x + \partial v/\partial y)\ (-\rho g)^{-1}\ dz \ . \qquad (4)$$

A.2 Dispersion Computations

Each particle emitted represents a growing cluster of particles until the size of the cluster exceeds the calculational grid spacing. This particle distribution can be viewed as the uncertainty in the particle's position. One can define those dimensions using the conventional notation of the standard deviation of the particle position in the horizonal σ_h and vertical σ_v directions. The rate of horizontal growth (line 12 in DEFAULT.CFG)

$$d\sigma_h/dt = 1853 \qquad (5)$$

is constant (Heffter, 1965), where σ_h is in meters and t in hours. However, the vertical growth rate,

$$(d\ \sigma_v\ )^2\ /dt = 2\ K_z\ , \qquad (6)$$

depends upon the local vertical diffusivity profile K_z, computed from the meteorological data as described in Appendix B. The upward growth is computed from the mixing at the k+1 index and the downward growth is computed from the mixing at the k index. Mixing coefficients are defined at the top of each model layer. Although this relationship between σ_v and K_z was considered valid primarily during stable conditions (Hunt, 1985), the values of K_z are so large during unstable conditions that the exact form of the equation is less important and it makes a useful approximation.

The particle, with its associated standard deviations for computational purposes, can be considered as a cylinder. Because the exact distribution of particles within that cylinder over larger travel times becomes more uncertain, the distribution is assumed to be uniform. The diffusion equations were initially defined for Gaussian distributions; therefore, one must define a relationship between the Gaussian and uniform "top hat" distribution, as shown on Fig. 1A.

At 1.54 σ (line 13 in DEFAULT.CFG), the ordinate of the Gaussian distribution is equal to the average value of the distribution; the areas above and below the horizontal dashed lines are equal. With this relationship, the horizontal radius R of the cylinder becomes 1.54 σ_h and the vertical height H is twice that or 3.08 σ_v.

The horizontal growth is assumed to be unbounded, but the vertical growth is only limited by the ground. The top of the model domain can act as a leaky lid depending upon the magnitude of the vertical mixing. The mixing is always largest within the boundary layer and those particles within the boundary layer are only constrained to that layer by the much smaller mixing coefficients in the free troposphere. However, some of a particle's mass may eventually mix out of the top of the model domain (Z_{mt}). A fraction of the particle's mass

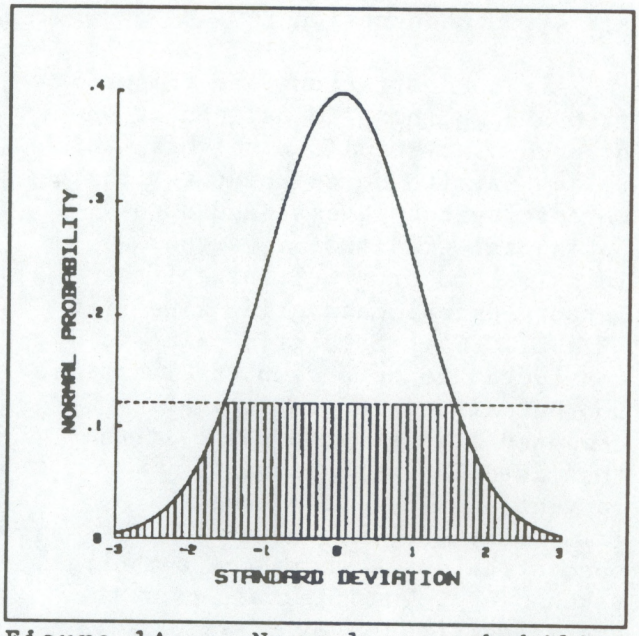


Figure 1A. Normal probability distribution. The dashed horizontal line indicates the ordinate value at which the shaded area equals the area above the line at 1.54 σ.

$$(Z_{mt} - Z_{cb})/(Z_{ct} - Z_{cb}) \quad (7)$$

remains within the model each time step when $Z_{ct}>Z_{mt}$. The remainder is lost. The subscripts denote the heights of the cylinder top (ct) and bottom (cb). Note that the denominator must equal 3.08 σ_v or

$$Z_{ct} = Z + 1.54\ \sigma_v$$

and

$$Z_{cb} = Z - 1.54\ \sigma_v\ . \quad (8)$$

The vertical distribution σ_v is redefined for particles when Z_{ct} exceeds Z_{mt} or for particles with Z_{cb} below zero. In those cases the new σ_v is redefined by

$$\sigma_v = (Z_{ct} - Z_{cb})/3.08\ , \quad (9)$$

using the new cylinder heights Z_{ct} and Z_{cb} where Z_{ct} is redefined at Z_{mt} or Z_{cb} at 0, respectively.

Particles at heights that exceed Z_{mt} are dropped from the calculation. Because the boundary layer (BL) depth can change with the meteorology, particles above the BL can at later times be below the BL. The condition of the BL depth occurring above Z_{mt} should be avoided by defining Z_{mt} well above the domain of interest, a large mass loss could occur through vigorous mixing out of the model top.

A.3 Air Concentration

Air concentrations are computed from a sampling grid defined at one or more user-specified heights, which do not have to be coincident with the meteorological levels, and on a horizontal grid that is either identical to or a multiple of the meteorological data grid (line 9 in DEFAULT.CFG). Each grid point is considered to be a sampling location, so that air concentrations are computed at that grid point, rather than as cell averages as in conventional Eulerian models. At grid point (i,j,k) the air concentration is where the sums are taken over $T_a/\Delta t$ intervals over the averaging time T_a; over A/R particle positions linearly interpolated over the distance advected (A) during the time step; and over p particles. In addition, the cylinder radius R with height H must intercept the grid point both in X,Y, and in Z. The integration of Eq. 10 is illustrated in Fig. 2A.

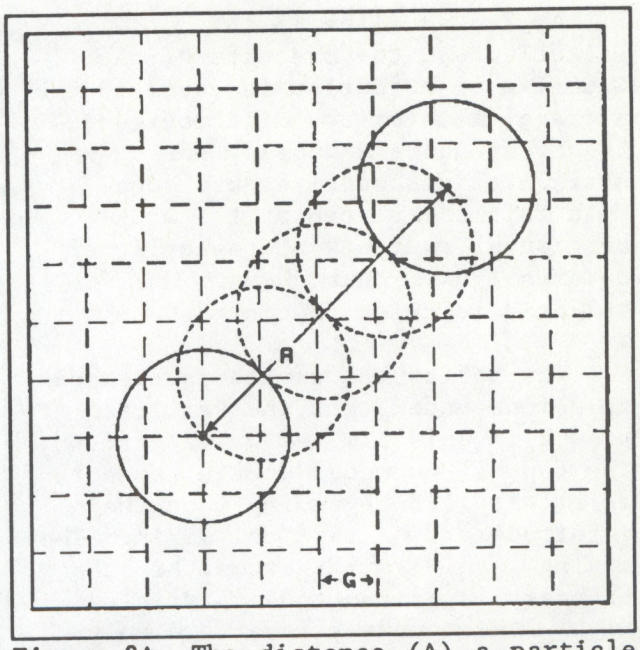


Figure 2A. The distance (A) a particle is advected during a time step. Three positions are interpolated so that the concentrations can be computed at all grid points at the interpolated (dashed) and initial and final positions (solid).

$$C_{i,j,k} = (\Delta t/T_a)(R/A) \sum_{1}^{T_a/\Delta t} \sum_{1}^{A/R} \sum_{1}^{p} (Q/(\pi R^2 H)) \ , \qquad (10)$$

The second of the three summations is necessary since particle positions may have to be interpolated to intermediate positions during a time step to avoid missing grid points if the cylinder radius is smaller than the advection distance. One additional constraint is that if the particle does not intercept any grid points during an advection step, it is assumed to pass over the nearest grid point. This avoids unrealistic gaps in the concentration field near the source where the particle radius is small.

A.4 Particle Management

When the growth of the cylinder extends either vertically or horizontally over two or more meteorological data points, then a single particle position can no longer adequately represent the advection-diffusion process. At this stage a particle is divided into two or more particles in which the sum of their masses equals the mass of the initial particle.

In the vertical dimension this process can be described as shown in Fig. 3A. Here the meteorological layers are shown by the long dashed lines. The sigma surface, where the meteorological parameters are calculated, is defined at the layer midpoint. When the growth of the cylinder is large enough to fully encompass at least two layers, that is Z_{ct} extends past Z_3 and Z_{cb} is below Z_1, then the particle Q_0 is divided into two particles of mass

$$Q_2 = Q_0 \, (Z_2 - Z_1)/(Z_3 - Z_1)$$

and

$$Q_3 = Q_0 \, (Z_3 - Z_2)/(Z_3 - Z_1) \; . \qquad (11)$$

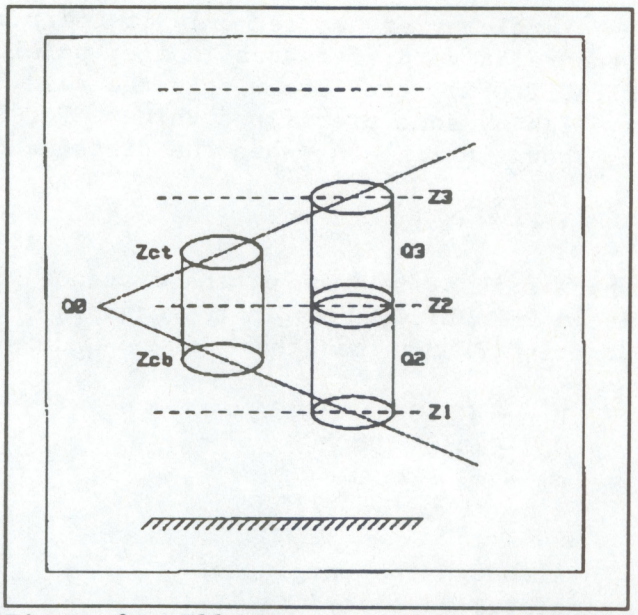


Figure 3A. Illustration of how a single particle Q0 splits due to vertical diffusion into two particle Q2 and Q3.

The new particles Q_2 and Q_3 have the same horizontal position as Q_0 but have an elevation equal to the layer midpoint. The σ_h value remains the same but the new σ_v value is proportioned exactly the same way as the mass.

The horizontal growth continues until the ratio of the cylinder radius R to the grid spacing G is greater than 1. This division ratio can be set to some other value in line 14 of DEFAULT.CFG. At this point (Fig. 4A) the particle is divided into four new particles, each with 0.25 of the initial mass. The new positions are orthogonal and equidistant from the old position by 0.5 R, with a σ_h value of 0.5 of the initial value but with the same σ_v value. The horizontal division is not important until longer travel times; given the constant growth rate, it would take 33 h for the first horizontal split to occur on a 85-km grid and 68 h on a 190-km grid.

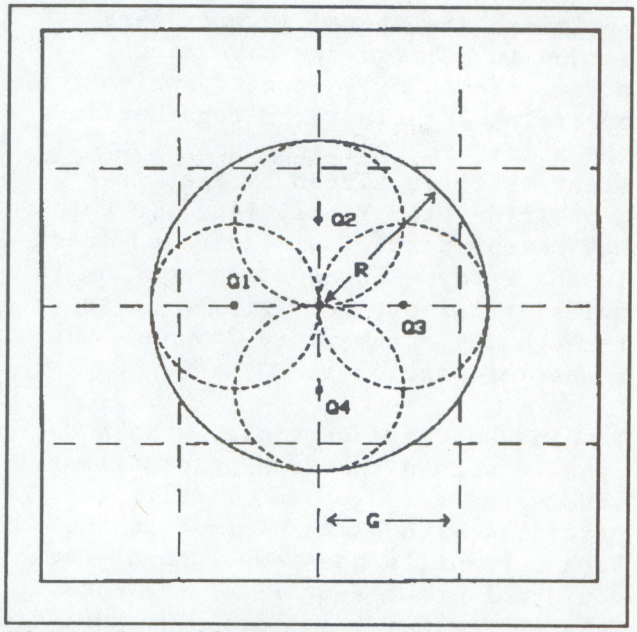


Figure 4A. Illustration of how a single particle with radius R splits due to horizontal diffusion into four particles each with radius R/2.

The key element to the practical application of this model is the elimination of duplicate particles. The generation of new particles, especially due to vertical diffusion, can quickly overwhelm even the fastest and largest computers.

Particles are merged only if their σ_h values (function of age) are equal (the relative differences in ages permitted to be merged is set in line 16 of DEFAULT.CFG), they are within the same layer, and their respective cylinders overlap by some predefined value. For instance, particles 1 and 2 are merged as shown in Fig. 5A, when the distance between their positions

$$| P_2 - P_1 | < f R , \tag{12}$$

where f is a fraction of the distance R. The default value of f is 1.0 (line 15 in DEFAULT.CFG) as in the example shown in Fig. 5A. The merged particle at position P_3 then has these mass-weighted attributes:

$$\begin{aligned} P_3 &= (Q_2+Q_1P_1)/(Q_2+Q_1) , \\ Q_3 &= Q_2+Q_1 , \\ \sigma_{h3} &= \sigma_{h2} = \sigma_{h1} , \\ \sigma_{v3} &= (Q_2\sigma_{v2}+Q_1\sigma_{v1})/(Q_2+Q_1) . \end{aligned} \tag{13}$$

Although the merging of coincident particles is in itself rather a trivial computation, the process can be cumbersome because there are no limits to the number of particles that can be generated or to their ages. Further, the particle positions are stored more or less at random in a large one-dimensional array. To quickly identify which particles are clustered together in the array, the particle position array is first sorted by age, level, X position, and Y position. In this way nearby particles will be adjacent in the array. The sorting routine is quite efficient, requiring n passes through the array where 2^n equals the number of particles.

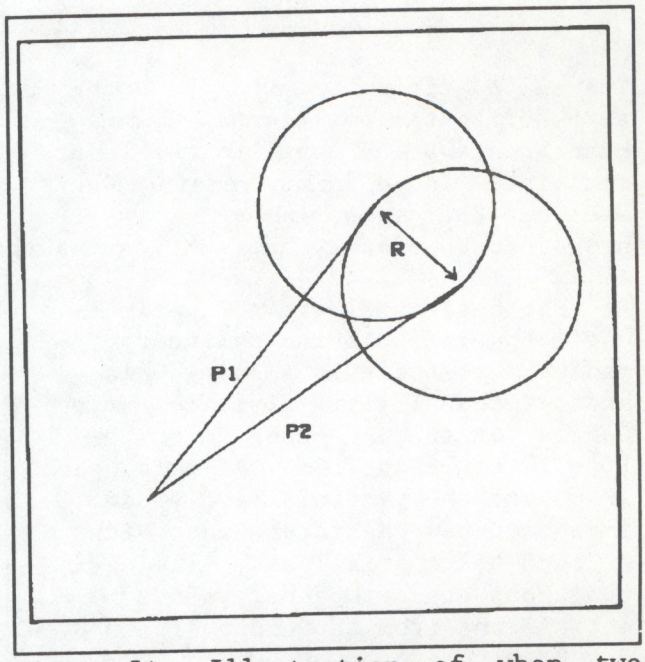


Figure 5A. Illustration of when two particles are merged into a single particle. It occurs when the difference between the vectors is less than R.

In addition, particles with a mass less than the 99th percentile mass value are dropped. If all particles with a mass less than the 99th percentile mass are summed, they would only represent 1% of the mass on the computational grid. This is similar to a 1% per day mass loss. The mass drop cut-off fraction can be set in line 17 of DEFAULT.CFG.

The particle merging occurs after the vertical diffusion division, thereby eliminating redundant particles at the same level. However, the horizontal division occurs after the merge calculation to avoid having a particle split and merge in the same time step.

APPENDIX B - HY-SPLIT METEOROLOGICAL PROCESSOR

There are three basic meteorological data sources anticipated for input to HY-SPLIT. These are NGM or MRF model analysis or forecast data, and rawinsonde data. Regardless of the source they are standardized into a similar format (discussed in Appendix D). However, each source may contain different variables on different surfaces. For instance, NGM data contain specific humidity on sigma surfaces, while the MRF data contain relative humidity on pressure surfaces. In general HY-SPLIT attempts to make the input data look as much like NGM data as possible. There is also a simple Ekman boundary layer model incorporated into HY-SPLIT to interpolate winds at levels below the lowest input sigma level. In particular this applies to NGM data where the lowest sigma level is about 200 m above ground. Additional meteorological levels between the surface and the first sigma level (200 m) can be specified, and the model will interpolate winds to those levels for subsequent transport and dispersion calculations.

B.1 NGM data sources

The NGM model forecast is initialized every 12 h (0000 and 1200 UTC), and the forecast fields are calculated to 48 h. ARL archives the forecast fields from 2 to 12 h at two hour intervals. The output interval of the forecast fields can vary from 1 to 6 h. The archived model output can be available on as many as 16 sigma surfaces at the midpoints of layers that vary in thickness from 35 mb at the surface to 54 mb at the model top. The routine data that are required for any calculation includes the three-dimensional state variables:

U, grid east-west wind speed
V, grid north-south wind speed
T, temperature
S, specific humidity.

The diagnostic vertical velocity W is optional for HY-SPLIT. As noted in Appendix A if not available, it is computed from the vertical integration of the horizontal velocity divergence. In addition, the following two-dimensional variables are required:

P_0, surface pressure (mb)
F_h, sensible heat flux at the surface (W m^{-2})
F_m, surface momentum exchange (kg m^{-2} s^{-1})
Z_{ml}, mixed layer depth (m).

Although other variables are also available, only these will be discussed here because they are used to develop the mixing coefficient profiles used in the dispersion calculations.

At each grid point the hydrostatic equation, $dZ = -dP/\rho g$, is integrated to convert the model layers defined at sigma surfaces to heights using the local

virtual temperature where R is the universal gas constant,

$$T_v = T/(1 - 0.608\ S) \quad . \tag{1}$$

The air density is computed from

$$\rho = M\ R^{-1}\ T_v^{-1} \quad , \tag{2}$$

where M is the molecular weight of dry air, T is temperature, and S is the specific humidity. The specific humidity is then replaced by the relative humidity

$$R_h = S\ P\ /\ (0.622\ e_s) \quad , \tag{3}$$

where the saturation vapor pressure (e_s in mb) is computed from

$$\exp[21.4-(5351/T)] \tag{4}$$

with T in Kelvin.

Rather than using the number of sigma layers within the mixed layer, reported by the NGM to compute the mixed layer depth, the depth is computed directly from the potential temperature profile at each grid point. The potential temperature is computed from the virtual temperature through

$$\theta = T_v\ (1000/P)^{0.286} \quad . \tag{5}$$

The mixing depth computation then follows the method of Heffter (1980) by computing the height at which the change in potential temperature from the base of the stable layer first exceeds two degrees. A stable layer is defined as a layer in which the potential temperature gradient exceeds 5°C per kilometer. The variation introduced here is that if a stable layer is not found with the first criterion, it is relaxed by one degree (to 4°/km) with each iteration. Three iterations are permitted before the mixed layer defaults to the model top.

The vertical mixing profile is determined by first computing the Monin-Obukhov length from the temperatures and velocities at the first

$$L = u_*^2\ T_v/k\ g\ \theta_* \quad , \tag{6}$$

model sigma level above ground. Von Karman's constant k is assumed to be 0.4 and the friction potential temperature

$$\theta_* = -F_h\ /\ \rho\ C_p\ u_* \quad . \tag{7}$$

Here C_p is defined as the specific heat at constant pressure and the surface friction velocity where the velocity (u) and air density (ρ) are at the first

$$u_*^2 = F_m\ u_1\ /\ \rho_1 \quad , \tag{8}$$

sigma level. It is assumed that the height of the constant flux layer Z_s always equals the first model sigma level. These sigma levels exclude those that may be defined for interpolation purposes. At the top of the surface layer the vertical mixing coefficient

$$K_z = k\, u_* Z_s / \phi \quad . \tag{9}$$

The normalized velocity profiles ϕ are taken from Businger (1973) such that when

$$L < 0 \;:\; \phi = (1 - 16\, Z_s/L)^{-0.25} \quad , \text{ and when}$$

$$L > 0 \;:\; \phi = (1 + 4.7\, Z_s/L) \quad . \tag{10}$$

Two methods are used to calculate the vertical mixing coefficient profile. In the first method, the O'Brien (1970) interpolation formula is used to derive the K_z profile to the top of the mixed layer. From the mixed layer top to the top of the model a small value of 0.1 $m^2\ s^{-1}$ is used for K_z. The second method is introduced to incorporate local stability measures above the mixed layer. Because the above technique applies only to turbulence generated by a boundary layer from surface-based momentum and heat flux values, a bulk Richardson number

$$R_i = g\, d(\ln \theta)/dz\ (du/dz)^{-2} \tag{11}$$

is calculated for each sigma level, and where R_i must be $> = -1$. Following the technique used in the NGM model calculation (Phillips, 1986), a vertical mixing coefficient is calculated assuming an arbitrary maximum value of 30 $m^2\ s^{-1}$ so that

$$K_z = 30/(2+R_i) \quad . \tag{12}$$

The final K_z value at any grid point is the maximum value obtained from either of the two methods. In this way, if significant wind-shear-induced turbulence is generated at night or above the boundary layer, the particle dispersion calculation will reflect the appropriately higher mixing rate.

The resulting vertical mixing coefficient profile is then limited to the range of 0.1 to 30 $m^2\ s^{-1}$. Values at each model level that are less or more than the permitted range are set to the limits.

B.2 MRF data sources

When the data source is from the MRF several alternative calculation paths are followed. The primary difference between the MRF and NGM is that data are on pressure rather than sigma surfaces, and no surface heat or momentum fluxes are available. MRF humidity data is already reported as relative humidity, so no additional conversions are required. Further the reported temperature data have been converted to virtual temperature. The effect of these differences is that the vertical mixing coefficient is computed only through the bulk Richardson number method and the mixed layer depth is estimated from data that

have a rather large vertical spacing.

B.3 Rawinsonde data sources

The processing of rawinsonde data for model input is accomplished through a pre-processor program discussed in considerable detail in Appendix C. The data are gridded according to the format described in Appendix D. The structure of the data output by the rawinsonde pre-processor program looks very much like NGM data in terms of the variables generated. The program accepts as input, rawinsonde or surface data, or a combination of the two. Options are available to process only wind soundings or include both winds and temperatures. The former would be used for pibal observations or perhaps profiler sounding data.

B.4 Boundary Layer Ekman Interpolation

For some applications it is necessary to have some finer resolution in the layers near the ground than what is available from the standard data sources. For the application discussed here one can use the previously computed Monin-Obukhov Length, vertical mixing coefficient, and estimate of surface roughness to compute the wind profile in the lowest layers of the model. Following Van Ulden and Holtslag (1985) one can compute the wind speed at any height below Z_1 from

$$U(Z) = U(Z_1) \frac{[\ln(Z/Z_0) - \psi_m(Z,L) + \psi_m(Z_0,L)]}{[\ln(Z_1/Z_0) - \psi_m(Z_1,L) + \psi_m(Z_0,L)]} \qquad (13)$$

and where the stability functions are given by

$$\psi_m = (1 - 16\ Z/L)^{0.25} - 1, \text{ and for } L<0$$

$$\psi_m = -5\ Z/L, \text{ for } L>=0\ . \qquad (14)$$

The roughness length, Z_0, is obtained from a file derived from global terrain height data which represents the terrain complexity within a grid square, rather than the land-use roughness. Limitations on the range of applicability of the similarity profiles require $Z_0 < |L| < U_*/f$, where f is the Coriolis parameter.

The wind direction profile is computed by fitting an Ekman profile to the Z_1 wind direction over a layer implied by the vertical mixing coefficient. The departure of the wind direction with height from the geostrophic direction, in radians, is defined by

$$A(Z) = \pi/2 - \arctan\ [\exp(aZ)\ \sin(aZ)^{-1} - \cot(aZ)]\ , \qquad (15)$$

where $a = (f/2K_z)^{0.5}$ and $a<\pi Z_1$. That is, the height of the Ekman layer should be no less than the first sigma level of the NGM. The wind direction at any height below Z_1 is then

$$D(Z) = D(Z_1) - A(Z) + A(Z_1) \quad . \tag{16}$$

With this definition the derived wind direction profile must match the wind direction at S_1. The above technique can be applied to data from the NGM or MRF. However, the output from these models should include at least one level within the boundary layer and a prediction of surface heat and momentum fluxes. As noted in section B.1 the fluxes are used to compute the mixing coefficient. In the case of MRF data the mixing coefficient calculation defaults to the value obtained from the bulk Richardson number method.

APPENDIX C - RAWINSONDE DATA PREPROCESSOR

C.1 General Program Structure

The meteorological preprocessor (*WT2GRID*) generates a time series of gridded observations from rawinsonde data and optional surface data, if available. Rawinsonde observation frequency can be at any time interval, but the program works best with at least two observation times per day. Near regions where four soundings per day are made, the spatial interpolation limits the influence of those locations to nearby grid points.

The importance of more frequent (greater than twice-daily) sounding data cannot be overemphasized. With only two soundings per day, it is suggested that more frequent surface observations be included to provide more realistic temporal variations of the surface energy budget. Otherwise linear interpolation between the two standard times may result in missing most of the diurnal cycle. The more frequent surface data are used to alter the low-level temperature profile, which then affects the stability and resulting surface fluxes of heat and momentum.

Input meteorological data are stored in three internal buffers to permit temporal interpolation between 6 or 12 hour observation intervals. Buffer-1 contains data from the previous time, while buffer-2 contains the data 6 hours later. The current data interpolation time falls between these two times. Buffer-3 contains the data for 12 hours after buffer-1. If the interpolation is occurring in a spatial region that does not contain any 6-hourly data, then the temporal interpolation occurs between buffers 1 and 3, otherwise it is between 1 and 2. In practice this means that if you want to grid data properly to the end of any one day it is necessary to have at least the data for the first observation time of the next day available in the input meteorological data file.

The output of the program is to a file that is comparable to the gridded output from the NGM discussed in Appendix D. Surface fields such as pressure, sensible heat flux, are followed by the winds, temperature, and moisture at each level above ground.

C.2 Vertical Gridding

Rawinsonde data above an observation point are first linearly interpolated at the designated vertical grid resolution to the top of the model at the nearest horizontal grid point. Wind direction and speed are converted to components relative to the polar stereographic grid. Temperature and pressure are directly interpolated to the vertical grid while dew-point is first converted to wet bulb potential temperature and then interpolated to the grid.

The original sounding is used to estimate the mixing depth, assumed to be the height of the base of the first elevated temperature inversion (Heffter, 1980). An inversion is defined as the height at which the potential

temperature increase within a stable layer first reaches 2°C. A stable layer is when the potential temperature increases by at least 5°/km. If no inversion is found the first time two additional passes are made with less restrictive stable layer definitions (4°C and 3°C per km).

The vertical levels are defined as sigma levels, fractional distances from the surface (1) to the top of the atmosphere (0) in a data statement in the main program. For subsequent vertical stability calculations it is good to have a level near the ground and one near the top of the constant flux layer (about 50 to 100m above ground). Subsequent levels can be designated at any interval. It is not necessary to output the additional lower levels in the final gridded data set as one of the constants set in the main program is the first data level to output. The lower levels may be omitted if one wants to generate a data set that looks identical to the NGM data or perhaps to elimate the influence of unrepresentative surface level winds.

C.3 Vertical Stability

At this point the sounding is further analyzed to determine the stability. The method follows that of Pielke and Mahrer (1975) in which equations for the Monin-Obukhov length, friction velocity, and surface friction potential temperature are solved by iteration using the surface layer flux relations of Businger (1973). With the variable $\xi = z/L$, the Obukhov length L, surface friction velocity u_*, and the surface friction potential temperature θ_* are given by

$$L = \theta \, u_*^2 \, (k \, g \, \theta_*)^{-1}$$

$$u_* = k \, u \, (\ln z/z_o - \psi_m + \psi_{mo})^{-1}$$

$$\theta_* = k(\theta - \theta_{zo}) \, (\ln z/z_o - \psi_h + \psi_{ho})^{-1} \, , \qquad (1)$$

where the "o" subscript refers to values at height z_o, the aerodynamic roughness length. The equations for the normalized wind (m - momentum) and temperature (h - heat) profiles are given in the table below:

Table 1C. Functions for normalized profiles of momentum and heat.

Parameter	$\xi>0$	$\xi\leq0$
ϕ		$(1 - 16 \, \xi)^{¼}$
ψ_m	$-5.0 \, \xi$	$\phi - 1$
ψ_h	$-5.0 \, \xi$	$2 \ln[\, 0.5(1+\phi^2) \,]$

The equations are solved iteratively for u_* until the variation is less than 25% between iterations or up to a maximum of five iterations. At this point the sensible heat flux (H) and momentum exchange coefficients (E) are computed through where the wind velocity and density are defined at the lowest

$$H = - \theta_* \rho C_p u_* \text{ , and}$$

$$E = u_* \rho u^{-1} \text{ ,} \qquad (2)$$

output level of the gridded data. The heat flux and exchange coefficient are then used by the HY-SPLIT meteorological processor (Appendix B) to compute the vertical mixing coefficient at each level and grid point.

C.4 Horizontal Gridding

After all the rawinsonde measurements are processed and assigned to the grid point nearest to the observation site, the data at the remaining grid points are interpolated from the grid points containing the rawinsonde data, using a conventional weighting (inverse distance squared). From rawinsonde observations taken either every 6 or 12 h, the gridded data are then linearly interpolated at intermediate intervals as frequently as desired.

A variable scan radius is used in the gridding routine, such that data from the off meteorological times (0600 UTC and 1800 UTC), which are not as spatially dense, are gridded first in a one pass scan. An interpolated value is generated if meteorological data are within the scan radius of that grid point. Grid points without nearby meteorological sites remain with missing values. These missing values at locations away from the off time data stations are filled by temporal interpolation from the primary 0000 and 1200 UTC observation times. Missing grid point data are not permitted at the primary times. If missing grid points remain after the first pass, the scan radius is incremented by the initial radius for the second pass. This process continues until all grid points have a value or until the scan radius equals half the grid dimension. At that point an error message will stop the process.

C.5 Optional Surface Observations

If surface observations are available, an additional step can be implemented. Because the surface data are taken more frequently over a much denser spatial network, these data can be used in a variety of ways. One of the most uncertain aspects of the model calculation is the temporal variation of the vertical mixing coefficient between two daily rawinsondes. When surface observations are available, as the interpolated fields are calculated, the lowest level interpolated temperature is replaced by the surface temperature observation. The stability is then recomputed as before, and new vertical mixing profiles are calculated.

The surface data input program is designed to work only with a fixed number of primary surface stations that report at three hour intervals. These are identified in a data statement by WMO number. Limiting the number of sites prevents the uneven weighting accorded to regions with denser networks or stations that report only part of the day.

After the rawinsonde data have been interpolated in space and time, the surface observation of wind, temperature, precipitation, and moisture replaces the interpolated gridded data at the lowest data level. After horizontal interpolation to fill all the grid points, the vertical mixing routine is then called again and the stability is analyzed with the new surface observation driving the gradients of wind and temperature.

C.6 Vertical Motion

After the meteorological data are gridded at each interpolation time, vertical motions are estimated by assuming that the wet-bulb potential temperature θ_w is conserved during an air parcel's ascent (Byers, 1974; p. 132). This method is preferred over integrating the velocity divergence because small errors in rawinsonde derived winds can produce large errors in the divergence field. Therefore, following the motion along a trajectory, the total derivative of θ_w is zero and hence the local rate of change is due only to advection. If we ignore the diabatic effects in the boundary layer and assume the θ_w field is frozen in time for the duration of the transport model advection time step, then the vertical velocity is

$$W = (-u\, \partial\theta_w/\partial x - v\, \partial\theta_w/\partial y)\, (\partial\theta_w/\partial z)^{-1} \qquad (3)$$

In this case, W is the vertical velocity required to maintain an air parcel on the same θ_w surface as computed at each grid point at a particular observation time. Applying this vertical velocity will not result in true isentropic flow as defined by Danielson (1961), for it is based only upon the slope of the θ_w surface with no energy constraints. However, in the boundary layer, isentropic trajectories are frequently in error since $\partial\theta_w/\partial Z$ approaches zero in a well mixed atmosphere. The primary purpose of defining W in this way is to permit particle trajectories to maintain a more realistic flow near air mass boundaries, where large horizontal and vertical gradients of θ_w make the calculation of W more accurate. When the gradients are calculated, one value of $\partial\theta_w/\partial Z$ is computed below and one above the mixed layer by a least-squares linear regression of θ_w on height. The vertical velocity is then integrated to each level from the appropriate average value of $\partial\theta_w/\partial Z$ and the centered difference horizontal gradients. If the value of $\partial\theta_w/\partial Z$ is less than 0.001 K m^{-1}, then a well-mixed layer is assumed and W is set to zero.

The final vertical velocity is the sum of the above term and the total derivative of pressure defined by

$$\partial P/\partial t + u\partial P/\partial x + v\partial P/\partial y \; . \qquad (4)$$

C.7 Program Output

The final output of the meteorological preprocessor then contains one byte packed gridded fields of U, V, W, Q, and T, at user-specified heights and time intervals.

APPENDIX D - GRIDDED METEOROLOGICAL DATA FORMAT

The primary sources of archival data are from the National Meteorological Center's (NMC) Nested Grid Model (NGM) and from the Global Data Assimilation System, which uses the Medium Range Forecast model (MRF). These data are available from a variety of sources, usually in Office Note 84 (ON-84) format. Before the data are archived by ARL they are converted to the format discussed in this Appendix, rather than saving them in ON-84 format. The advantage is that our format is more compact and it can be directly used on a variety of computing platforms with direct access I/O. In addition to model generated gridded data, the rawinsonde preprocessor program discussed in Appendix C will generate a gridded data set matching the characteristics discussed below. Meteorological data in this format can then be read directly by the HY-SPLIT meteorological input subroutine without additional conversions. It is not necessary that all variables or levels be present for HY-SPLIT to be able to use the data. Depending upon the data source, NGM, MRF, or Rawinsondes, different combinations of fields and levels are available. The HY-SPLIT meteorological preprocessor subroutine (Appendix B) converts what is available from the input file to what the model needs for computational purposes.

D.1 Data Grids

In the following table each data grid is identified by the model that produced the data, an internal grid identification number, the number of West-East (X) and South-North (Y) grid points, the grid spacing (Δ) in time and space (true at the indicated latitude), the longitude to which the Y axis is aligned, and the pole position in grid units. The given pole position results in the lowest left grid point to have a value of (1,1).

Table 1D.--Structure and orientation of meteorological data grids

Model	ID	X	Y	Δ	Δ	True	Align	X	Y
Type	#	Max	Max	Hr	Km	Lat.	Lon.	Pole	Pole
NGM	00	65	56	02	91.45	60N	105W	25.5	84.5
NGM	01	28	20	02	182.9	60N	105W	10.75	39.25
MRF	02	65	65	06	381.0	60N	80W	33.0	33.0
MRF	03	65	65	06	381.0	60S	100E	33.0	33.0
LFM	04	53	45	06	190.5	60N	105W	27.0	49.0
NGM	06	33	28	02	182.9	60N	105W	13.25	42.75
PEG	07	33	33	06	91.45	60N	50E	17.0	99.0

The three primary sources of gridded meteorological data are illustrated in Figs. 1D - 3D. The center location of each grid point is represented by the "+" symbol and the lower left mark is at the (1,1) position. All of the meteorological data grids are based upon a polar stereographic projection. The HY-SPLIT code is also capable of processing data on an oblique stereographic projection. An oblique projection is the default when the grid spacing is 40 km or less.

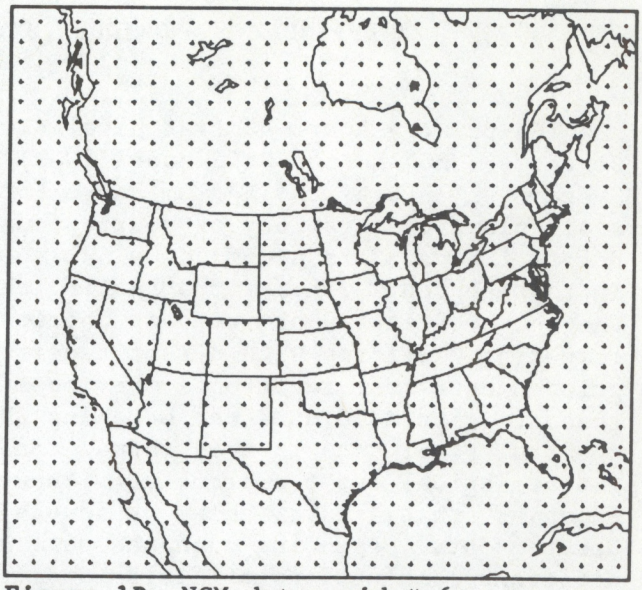


Figure 1D. NGM data grid # 6.

One special application, PEG (Persian Gulf), not shown here, is an example of some other output possibilities. In this case the MRF data was output on a special higher resolution grid on vertical sigma, rather than pressure surfaces, for a two month period during the summer of 1991.

Many different special grids can be derived from the primary data grids through the utility program *GAMDUP*. It is possible to extract a sub-grid from the larger grid to save the data only in the region of interest. In these situations it is necessary to make an additional entry into the METFILE.CFG file which describes the spatial domain of the new grid.

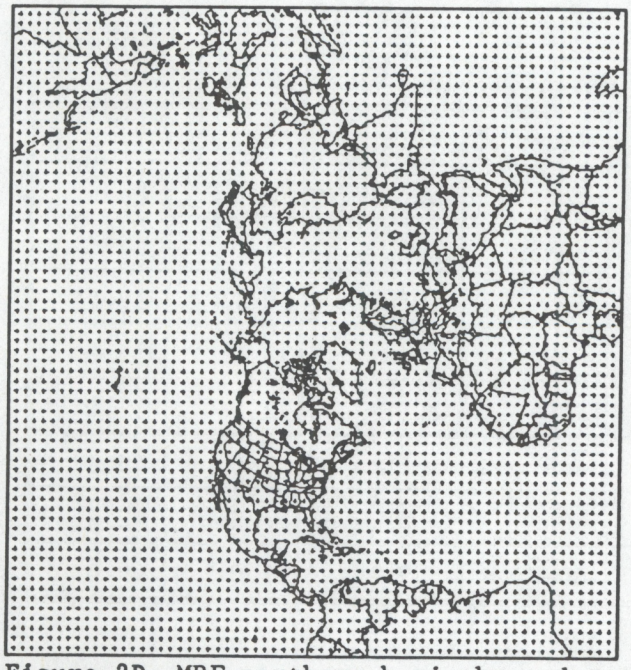


Figure 2D. MRF northern hemisphere data grid number 2.

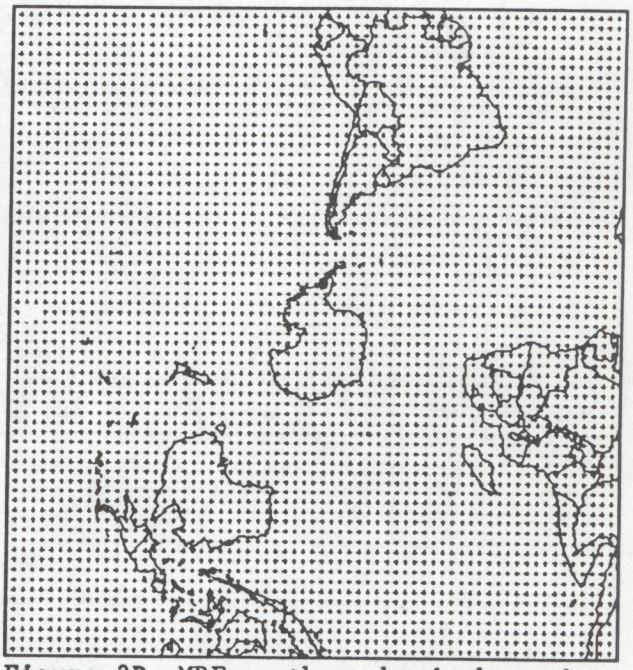


Figure 3D. MRF southern hemisphere data grid number 3.

D.2 Historical Archive

The various model data have been available with considerable gaps starting with the ANATEX experiment from January through March of 1987. The data availability is summarized below:

Table 2D.--Availability of meteorological data

Model Source	NGM	NGM	NGM	MRF	MRF	LFM	PEG
Grid Ident	00	01	06	02	03	04	07
Forecast				X	X	X	
Special					X		X
Jan-Mar 1987	X						
1989	X	X					
1990		X					
1991 to present			X	X	X		

In addition to the time periods noted for archival data, some data fields are also available on a "forecast" basis. Forecast fields are not archived and are only available operationally on the day the forecast is made. Special products, such as PEG, are available only by request and require initiating a procedure on the main-frame computer to make them available for routine use. These would normally be terminated after the special request is satisfied. The NGM and MRF data archives can be obtained from NCDC starting from January 1991 under identification TD-6140.

D.3 Meteorological Fields

Each archive data set has different fields available according to what is normally produced by the model and disk space limitations. The fields are identified by a description, the units, and a unique four character identification that is written to the header label at the beginning of each field. Data availability are identified by a two digit code. The first digit indicates if it is a surface level variable (S) or an upper level variable (U). The second digit indicates the order in which that variable appears in the file. The following table identifies the data fields available with the most common data grids.

Table 3D.--Meteorological parameters and their organization

Field Type	Units	Label	NGM	NGM	NGM	MRF	PEG
Grid Ident			00	01	06	2/3	7
Total Precip	m	TPPT	S1	S1	S6		S2
Snow Cover	0/1	SNOW	S2		S2		
Exchange	kg/m2/s	EXCO	S3	S2	S7		
Heat Flux	W/m2	HFLX	S4	S3	S8		
Water Flux	kg/m2/s	WFLX	S5	S4	S9		
Soil Temp	K	TGRD	S6				
Sfc Temperature	K	TMPS				S2	
Sfc Pressure	mb	PRSS	S7	S5	S10	S1	S1
Mixed Layers	Sigma	MXLR	S8	S6	S11		
Terrain Height	m	SHGT	S9		S3		
Sea Level Press	mb	MSLP	S10		S4	S3	
Ice Covr Water	0/1	ICWT			S1		
Convc Precip	m	CPPT			S5		
U Wind	m/s	UWND	U1	U1	U1	U1	U1
V Wind	m/s	VWND	U2	U2	U2	U2	U2
Omega (W wind)	mb/s	WWND	U3	U3	U3	U5a	
Specific Hum	kg/kg	SPHU	U4	U4	U4		U4
Temperature	K	TEMP	U5	U5	U5	U4	U3
Relative Hum	%	RELH				U6b	
Pressure Hgts	m	HGTS				U3	

a - Vertical velocities available only through 100 mb.
b - Relative humidities available only through 300 mb.

D.4 Vertical Structure

The NGM data are output on sigma surfaces relative to model terrain while the MRF data are output on the mandatory pressure surfaces, except for the special output developed for PEG (07), which is also on sigma surfaces. The archive vertical structures are summarized below:

Table 4D.--Vertical levels available in each data set

Sigma	NGM	NGM	NGM
Grid	00	01	06
.022	X		
.146	X		
.286	X		
.434	X		X
.509	X		X
.582	X		X
.653	X		X
.721	X	X	X
.785	X	X	X
.844	X	X	X
.897	X	X	X
.943	X	X	X
.982	X	X	X

Sigma	MRF
	7
.497	X
.594	X
.688	X
.777	X
.856	X
.920	X
.960	X
.981	X
.995	X

mb	MRF
	2/3
50	X
70	X
100	X
150	X
200	X
250	X
300	X
400	X
500	X
700	X
850	X
1000	X

The data file will contain the data in synoptic time sequence, without any missing records (missing data will be represented by negative 1 in the forecast hour field and/or NULL in the variable identification field). Therefore, it is possible to position randomly to any point within a data file. At each time period the surface level data are followed by all the variables in each level from the ground up. The MRF data is also organized in synoptic sequence. However, for each time period the Northern Hemisphere data come first, followed by the Southern Hemisphere.

D.5 Data Grid Unpacking Procedure

The data grid is packed and stored into one byte characters. To preserve as much data precision as possible the difference between the values at grid points is saved and packed rather than the actual values. The grid is then reconstructed by adding the differences between grid values starting with the first value, which is stored in unpacked ASCII form in the header record. To illustrate the process, assume that a grid of real data, R, of dimensions i,j is given by the below example.

Table 5D.--Grid structure of packed data

1,j	2,j	....	i-1,j	i,j
1,j-1	2,j-1	....	i-1,j-1	i,j-1
....	....	....	....	....
1,2	2,2	....	i-1,2	i,2
1,1	2,1	....	i-1,1	i,1

The packed value P at a grid point (m,n) within the (i,j) domain, is then given by

$$P_{m,n} = (R_{m,n} - R_{m-1,n})\ 2^{(7-N)}\ , \qquad (1)$$

where the scaling exponent

$$N = \ln \Delta R_{max} / \ln 2\ . \qquad (2)$$

The value of ΔR_{max} is the maximum difference between any two adjacent grid points over the entire array. It is computed from the differences along each m index holding n constant. The difference at index (1,n) is computed from index (1,n-1), and at 1,1 the difference is always zero. The packed values are one byte unsigned integers, where values from 0 to 126 represent -127 to -1, 127 represents zero, and values of 128 to 254 represent 1 to 127. Each record is then equal in bytes to the number of array elements plus 50 bytes for the label information. The 50 byte label field precedes each packed data field and contains the following ASCII data.

Field	Format	Description
Year	I2	Greenwich date for which data valid
Month	I2	"
Day	I2	"
Hour	I2	"
Forecast	I2	Hours forecast, if not initialization
Level	I2	Level from the surface up (see D.4)
Grid	I2	Grid identification (see D.1)
Variable	A4	Variable label (see D.3)
Exponent	I4	Scaling exponent needed for unpacking
Precision	E14.7	Precision of unpacked data
Value 1,1	E14.7	Unpacked data value at grid point 1,1

An example fortran program to unpack the data array is given below. Here the packed data array is in the variable QPACK and the unpacked real data array is returned in variable RVAR. NX and NY are the number of grid points in the horizontal and vertical directions, respectively. The variable NEXP and VAR1, are the packing exponent and value of the field at the 1,1 grid point.

```
SUBROUTINE UNPACK(RVAR,QPACK,NX,NY,NXY,NEXP,VAR1)

CHARACTER*1 QPACK(NXY)
REAL*4 RVAR(NX,NY)
SCALE=2.0**(7-NEXP)
VOLD=VAR1
INDX=0
DO J=1,NY
   DO I=1,NX
      INDX=INDX+1
      RVAR(I,J)=(ICHAR(QPACK(INDX))-127.)/SCALE+VOLD
      VOLD=RVAR(I,J)
   END DO
   VOLD=RVAR(1,J)
END DO
RETURN
END
```

APPENDIX E - DEFAULT.DAT INPUT FILE DESCRIPTION

Each input line of the DEFAULT.DAT file is numbered in sequence, followed by an identification, and flag identifying the field as character (C), integer (I), or real (R).

---

(1) TRAJECTORY TIME STEP (I)

Integration time steps can vary from 1 hr to the frequency of the input meteorological data in whole hour intervals. Larger time steps may be selected to reduce computation times.

(2) DIRECTION (C)

The calculation direction can be selected for forward (FWRD) or backward (BACK). Note that concentration output is not available in the backward mode--only trajectories.

(3) VERTICAL MOTION (C)

The vertical motion calculation can be made using either isobaric (ISOB) coordinates, isosigma (ISOS) coordinates, the omega vertical velocity field from the MRF or NGM provided with the input data (DATA), or through vertical velocities calculated from the horizontal velocity divergence (DIVG). In the isobaric case a trajectory maintains the same pressure but may be displaced relative to the local terrain; while in the isosigma case a trajectory maintains the same sigma level relative to the local terrain, but may of course change its pressure level. In the latter two options either may occur.

(4) STARTING MONTH (I)

This is the month in which the model run will start. The starting time is used to position the meteorological input file to the correct initial date. A value of zero will default to the meteorology file month and cause the subsequent starting day and hour to be interpreted as relative to the first data observation in the input file.

(5) STARTING DAY (I)

The starting day is the forward trajectory starting point or in backward mode it is the termination time of the forward trajectory. A value of zero will default to the meteorology file starting day.

(6) STARTING HOUR (I)

Emissions or trajectories will start on the hour selected. All times are in Greenwich. Setting a negative start hour results in no emissions but the input file will be positioned to that hour. That option is valid only with starting endpoints read from disk.

(7) DAYS TO RUN MODEL (I)

The model will run for the number of days from 0000 UTC beginning on the start day. Only whole days are permitted. If a trajectory is started in the middle of a day it will terminate that day unless more than one run day is specified.

(8) METEOROLOGY FILE NAME (C)

Only the prefix name, usually month\year, is required as the suffix (.bin) will be assumed. If another suffix is specified it will be used instead of the default value. The directory path is given in file DEFAULT.CFG. Subsequent end of files encountered during the model run require dynamic entry of a complete file name.

(9) ORIGIN LATITUDE (R)

This is the emission starting point for all particle trajectories in degrees and decimal fraction. Use negative values for southern hemisphere starting locations.

(10) ORIGIN LONGITUDE (R)

West longitudes are positive, east longitudes are negative, and as with latitude it is in degrees and decimal fraction.

(11) ORIGIN HEIGHT (R)

Starting height is specified in meters above model terrain and not the actual local terrain. Optionally the starting height may be specified in absolute pressure units (mb). In that case the pressure level is directly followed (no space) by the letter P.

(12) SOURCE EMISSION RATE (R)

The source term is always specified in mass units per hour, regardless of the hours of emission or model time step. The units of mass are not relevant because output values are in mass units per cubic meter. A source term of zero results in the release of one particle of unit mass--or a simple single trajectory calculation. No concentration or dispersion calculations are performed when this option is selected.

(13) NUMBER OF HOURS OF EMISSION (I)

Particles will be emitted continuously for the number of hours specified in this field for any one emission repeat interval.

(14) EMISSION REPEAT INTERVAL (I)

The emissions can be repeated for the number of hours of emission at the repeat cycle interval given in hours. For instance if you want 3 hours of emission every 24 hours starting at 1200 UTC set this field to 24, the previous one to 3, and the starting time at 12.

(15) OUTPUT and/or AVERAGING PERIOD (I)

All output tables and maps: printer, screen, or graphics; will occur at this interval in hours. For concentration output this field specifies the averaging interval. All output maps are marked with the time at the start of the period. Trajectory output is always identified by the origin start time regardless of how many maps output.

(16) OUTPUT OFFSET TIME/START HOUR (I)

The value in this field specifies the UTC hour that the averaging or output interval counters will start. For instance if you want 24-h concentration output, but from 1200 to 1200 of the following day set this field to 12. No output will be printed for the first incomplete averaging period.

(17) CONCENTRATION AT INDEX (I)

Concentrations are calculated at a minimum of one level. However, only one level can be output in any one simulation and that level is selected by this parameter. To determine if your version was compiled for multi-level concentrations, the value of KCX in the GRIDVAL.DAT file would be greater than one. In this entry select the index number of the level desired for model output. A selection of zero in this field results in output of the deposition field if the appropriate subroutine was included in the compiled version.

(18) HEIGHT OF THE CONCENTRATION LEVEL (I)

In general the heights of each concentration level default to the corresponding meteorological sigma level. Interpolated sigma levels are included if that option was selected in the DEFAULT.CFG file (line 4). However, by selecting a value greater than zero in this field you can override the height above ground that corresponds with the previously selected index. Other levels remain unaltered. See file DEFAULT.CFG for a listing of sigma levels.

(19) ENDPOINTS TO/FROM DISK (C)

Depending upon the option selected you may WRITE all particle positions to disk at the end of the run. The next time you start the model you can READ the endpoints file and essentially continue the same run and write again if MOD was selected. If you are doing concentrations it is recommended that the end of a sampling period correspond to the end of the run. Concentration arrays are not reinstated to the previous termination values. Selecting the STEP option permits endpoints to be output to disk file ENDPTS.ASC at the interval selected for model output (entry 15).

(20) CONCENTRATION OUTPUT TO DISK (C)

Values on the concentration grid can be saved (WRITE) to a disk file (MDLCON.BIN) at the output interval. Regardless of the setting in line 18, all compiled levels of the concentration array are written to the data file. The number of levels written to disk can be modified by adjusting the array size in the DEFAULT.CFG file (line 8). The MDLCON.BIN file can be read later by other graphics codes for display purposes without having to recompute trajectories. MODify adds to the end of a previously created file.

(21) MAP OUTPUTS- TRAJectories SNAPshots CONCentration (C)

Snapshots of the particle positions can be displayed at the output interval by selecting SNAP or the cumulative trajectory of each particle can be displayed by selecting TRAJ. The selection of TRAJ for output is independent of the selection of trajectory computation through setting

the source term to zero. In the former case although concentrations are being determined by the advection and diffusion of many particles their trajectories can be displayed. However, in the latter case, if only one particle trajectory is calculated, then a trajectory display is the most appropriate output. CONCentration output is given at each grid point.

(22) OUTPUT GRAPHICS MAPS (C)

Graphics option NONE means that the previously selected maps will be displayed on your standard output device in ASCII. No special subroutines are required, but no map backgrounds are available with this option. Set your printer for compressed print for ASCII maps as they default to 132 columns unless the DEFAULT.CFG file is modified. A graphics option of YES provides a real-time display of the same ASCII maps to the screen as they are being calculated. However, with the graphics option on, error messages and prompts cannot be displayed, and are saved to a file called HYSPLIT.MSG. Please check this file for messages at the end of a run.

(23) OUTPUT ASCII MAP DEVICE SELECTION (C)

The device selection is the default device for ASCII line printer style output maps (needed if you only have a mainframe without other graphics capabilities). If you don't care about hard-copy without the map backgrounds or are getting run-time graphics select the NUL device (no file created). Other options are the screen (CONsole), LPT (standard printer), or output to a FILE which will always be named PRINT.ASC. Default output directories are set in DEFAULT.CFG (line 26).

(24) MAP BOUNDARIES TOP LATITUDE (R)

The orientation of all output maps is determined by these boundaries. The top latitude is used to set the upper right corner of the map. Zeros in the map boundary fields will cause the program to determine the most appropriate map dimensions.

(25) MAP BOUNDARIES BOTTOM LATITUDE (R)

The bottom latitude is used to set the lower left corner of the map.

(26) MAP BOUNDARIES RIGHT LONGITUDE (R)

The right boundary is adjusted to maintain the correct aspect ratio of the proper polar stereographic projection. It usually will be much further to the right than what you specified. The lower left and upper right corners in conjunction with the output media are used to determine the aspect ratio and scaling. The right boundary of the map then floats to fill the rest of the page.

(27) MAP BOUNDARIES LEFT LONGITUDE (R)

The left longitude is used in conjunction with the bottom latitude to set the left boundary of the map.

APPENDIX F - DEFAULT.CFG INPUT FILE DESCRIPTION

Each input line of the DEFAULT.CFG file is numbered in sequence, followed by an identification, and flag identifying the field as character (C), integer (I), or real (R).

---

(1) METEOROLOGICAL SUB-GRID X-AXIS LIMITS (I)

The sub-grid selection is required only if the model is compiled, due to core limitations, for a smaller computational data grid than what is available on the input data file. If the default sub-grid, the dimensioned limits from the lower left corner of the input data, are in the proper spatial domain, then default values of zero will be sufficient. If the sub-grid needs to be shifted, then at least the lower left corner position must be specified. If you don't have a clue as to what value to put in, run the model for your source location, (turn off run-time graphics) and the program will tell you what value to enter for the corner to get you selected source location to be in the center of the meteorological sub-grid.

(2) METEOROLOGICAL SUB-GRID Y-AXIS LIMITS (I)

See x-axis for instructions.

(3) METEOROLOGICAL VERTICAL SUB-GRID LIMITS (I)

Similar to the horizontal, one may select any number of consecutive levels from the input data file. A default value of zero loads whatever number of levels from the input data file from the bottom up until the compiled dimensioned limits have been reached. Otherwise any range within the vertical domain and compiled array limits may be selected.

(4) NUMBER OF INTERPOLATED SURFACE LAYERS (I)

One may specify additional levels below the lowest meteorological level available in the data file. Winds at these levels are interpolated through an Ekman/similarity approach. It works best when surface momentum and heat fluxes are available from the input data file (usually NGM).

(5) HEIGHT OF INTERPOLATED LEVELS IN METERS ABOVE AGL (R)

Specify the height of each interpolated level. They all should be below the first model sigma level.

(6) CONCENTRATION SUB-GRID X-AXIS LIMITS (I)

For similar reasons as with the meteorology it may be necessary to specify a sub-grid. These values are in the same units as the meteorological data, therefore, if you are unsure as to what to do, use the same values as above. If the horizontal spacing of the concentration grid is not the same as that of the meteorological grid (see line 9 below) you still specify the sub-grid in meteorological grid units. However, the compiled dimensions may be exceeded as the actual number of grid points within the sub-grid domain increases by the selected grid

factor. In that case it may be necessary to alter the ICX and JCX variables in the GRIDVAL.DAT file and recompile the code.

(7) CONCENTRATION SUB-GRID Y-AXIS LIMITS (I)
See x-axis limits.

(8) CONCENTRATION NUMBER OF VERTICAL LEVELS (I)
A zero defaults to the compilation maximum given in GRIDVAL.DAT (KCX). Use this parameter to control the size of the output concentration array MDLCON.BIN. Fewer concentration levels also increase computational speed.

(9) GRID SPACING MULTIPLIER AS CONC GRID PTS PER METEO GRID PT (I)
Normally the horizontal spacing of the concentration grid will be identical to the meteorological grid. However, one can obtain finer resolution be setting this value to some integer greater than 1. It is defined as the meteorological grid spacing divided by the concentration grid spacing.

(10) SOURCE MOLECULAR WEIGHT CONVERSION OF M/M3 to L/L (R)
Normally source term values are specified in arbitrary mass units per hour resulting in concentration output of mass units per cubic meter. If you prefer volume units (liter/liter) then specify the emissions in grams and set the appropriate gram molecular weight in this field.

(11) MASS INDEX TO USE ONLY WITH MULTI MASS SIMULATIONS (I)
You may have a compiled version for multiple species tracked at the same time. For instance (1)-SO2 and (2)-SO4, etc. In that case selecting the appropriate index sets all output for that species. The default value is 1.

(12) HORIZONTAL DISPERSION RATE (R)
The default dispersion rate 1853 m/hr represents the rate about which the distribution about each particle grows.

(13) SIGMA OF HORIZONTAL RADIUS FOR UNIFORM DISTRIBUTION (R)
The radius about a particle is assumed to default to 1.54 of the horizontal variance, the case of a uniform horizontal distribution (top hat).

(14) HORIZONTAL RADIUS PARTICLE SPLIT FRACTION (R)
When the ratio of the horizontal radius to the horizontal grid spacing exceeds this factor a single particle is split into four particles with the appropriate smaller radius and mass. The default value is 1.

(15) FRACTION OF RADIUS OVERLAP FOR CONVERGENCE (R)
If two particles occupy the same space they are merged if the distance between their centers is less than the above factor times the radius. The suggested default value is 1.

(16) TEMPORAL OVERLAP FRACTION BEFORE CONVERGENCE (R)
If particles are sequentially released at different times, they can be merged if the difference in release times over the travel time is less than the above fraction. The suggested default value is 0.15.

(17) DAILY MASS PURGE FRACTION OF TOTAL MASS (R)
One a day (at 2400 hrs UTC) the total mass on the computational domain is computed. The particle mass that represents the percent value noted here (default 1%) is determined from the cumulative mass distribution. All particles with mass less than this value are dropped. The suggested default is 0.01.

(18) MAXIMUM DURATION IN HOURS BEFORE TRAJECTORY TERMINATION (I)
Trajectories are deleted after the given number of hours. This parameter is especially useful if you are running multiple trajectories, say four per day over a 30 day simulation period, but you want each of the trajectories to terminate after 24 hours. The suggested default value is 999.

(19) HOURS MISSING DATA BEFORE ALL TRAJECTORY TERMINATION (I)
Missing meteorological data triggers a warning message, however, all computations continue until the next input cycle to see if the proper data are present. The persistence of old data will continue for the number of hours specified in this field, before dropping all computations. The suggested default value is 12.

(20) INITIAL SOURCE INDEX VALUE FOR CYCLED SOURCE TERM (I)
Each emission cycle, as specified by the repeat index in DEFAULT.DAT is numbered sequentially from 1. This value is written to the output file to identify concentrations associated with a particular emission when there are multiple emission cycles.

(21) MAXIMUM SOURCE INDEX FOR CYCLED SOURCE ONLY (I)
In addition to the field above, the source index can be used to limit the number of source repeat cycles, as specified in this field.

(22) MAPS LAT/LON LABEL INTERVAL IN DEGREES (R)
This is the label interval for latitude and longitude lines.

(23) MAXIMUM ASCII PRINT WIDTH OF HORIZONTAL CARRIAGE (R)
Normal ASCII printer maps require 132 columns at 10 characters per inch. If you only have a short carriage printer and no compressed print mode, you can set the maximum output length in inches.

(24) DIRECTORY INPUT FILES FOR CFG DAT TXT FILES (C)
The directory the model searches for all input files, except the meteorological data, is set in this field. The exception of course is this file, DEFAULT.CFG, which must be in the default directory. That is the directory from which the model is launched.

(25) DIRECTORY FOR METEOROLOGICAL DATA (C)
The meteorological data can reside in a separate directory. Note that all directory specifications must end with the slash, ie (\main\sub\). If the desired default directory is the home directory, it can be specified by a null field or dot in DOS or a ./ in UNIX.

(26) DIRECTORY FOR MODEL OUTPUT FILES (C)
All outputs, HYSPLIT.MSG, MDLCON.BIN, MDLCON.CFG, PRINT.ASC, ENDPTS.ASC, and ENDPTS.CFG, will go to this directory. Note that if you generate an output file that is used for input, it must first be moved to the input directory.

APPENDIX G - INSTALLATION, RUNNING, AND FILE FORMATS

G.1 Installation

The program and test files may come on one or more disks depending upon how much of the source code and additional meteorological data has been provided. It is packed using standard PKZIP routines and the main program disk contains a batch file that will install the model and unpack the data. This program will create appropriate sub-directories on any disk drive you select. HY-SPLIT is much easier to operate if it is installed to the hard disk. To install the program on drive C: in a directory off the root directory called HYSPLIT3, switch the default drive to the drive in which the floppy disk resides (ie A:) and then type:
INSTALL C: \HYSPLIT3 and press Enter. The following subdirectories and files will be created:

Subdirectory	Files	Description
EXECMDL	README	
	HYSPLIT.BAT	Batch file to run model
MDLCODE	HYMODEL.EXE	Compiled HY-SPLIT
	GRIDVAL.DAT	Compilation constants
	-------.FOR	Optional source code
CFGFILE	TEST00?.DAT	Test data DEFAULT.DAT
	TEST00?.CFG	Test data DEFAULT.CFG
	METFILE.CFG	Meteorological grids
	ROUGLEN.BIN	Aerodynamic roughness
	MODERN.FON	Run-time graphics font
	EZMPDAT	Map background file
METDATA	TESTNGM.BIN	Test NGM meteo data
	TESTMRF.BIN	Test MRF meteo data
UTILITY	GAMDUP.EXE	Archive management utility
	GAMGOP.EXE	Archive graphics output
	GAMPOP.EXE	Archive printer output
	GAM---.FOR	Optional source codes
	WT2GRID.FOR	Rawinsonde gridding code
	WT2GRID.INC	Rawinsonde include file
GRAPHIC	PLOTTER.BAT	Post processing batch file
	TRAJPLOT.EXE	Trajectory plotting pgm
	CONCPLOT.EXE	Qualitative concentrations
	GRIDPLOT.EXE	Quantitative concentrations
	GRID2STN.EXE	Grid to station conversion
	--------.FOR	Optional source codes
	KOLMAP.DAT	Colors definition table
	HYTEK.EXE	Tektronix emulator pgm

Subdirectory	Files	Description
	HYTEK.CFG	Tektronix configuration
	HYVIEW.EXE	Skew-T display
EDITORS	HYEDIT.EXE	DEFAULT.DAT/CFG text editor
	HYMAPS.EXE	DEFAULT.DAT map editor
	HYPICK.EXE	DEFAULT.DAT mouse editor
	HLPDAT.TXT	DEFAULT.DAT help file
	HLPCFG.TXT	DEFAULT.CFG help file

G.2 Running the Model with the batch file

Switch to the EXECMDL directory. The batch file HYSPLIT performs several operations depending upon the options that you select. The format is as follows:

HYSPLIT [config] [dat] [cfg] [map] [pic]

[config] The required prefix name for the .DAT and .CFG files that will be copied into DEFAULT.DAT and DEFAULT.CFG. The model searches the default files for the input parameters. To run the example case you would for example enter TEST005 in this field.

[dat] Invokes the editor for the DEFAULT.DAT file.

[cfg] Invokes the editor for the DEFAULT.CFG file.

[map] Invokes the mouse driven editor to set the source location and output map domain in DEFAULT.DAT.

[pic] Invokes the mouse driven editor to set various options in the DEFAULT.DAT file. Can be used instead of HYEDIT when only simple changes are required.

The options can be invoked in any order, upper or lower case. Most model input files are located in the CFGFILE directory. The files to be edited, files like TEST001.DAT and TEST001.CFG, are copied into the editors directory for editing and then copied back into the cfgfile directory. In addition, a copy of DEFAULT.CFG is placed in the MDLCODE directory. The directory from which the model is initiated requires the DEFAULT.CFG file to tell it where to find the other files.

You will see three different graphics screens that are used to edit the model input files, two are keyboard text editors and one is a mouse driven editor for setting the display map and source point. For this test simulation just press the ESC key or two-button mouse click, as appropriate, to exit each menu. In the future you can use the CTRL-I key to examine a help file that goes along with each model entry in the text editor. After the model starts you will be prompted to press any key to continue, this gives you a chance to

BREAK after editing the input files before starting the model simulation. During the simulation a real-time graphics display will follow with the calculation. After completion the model waits for ENTER to continue. The post-processing graphics programs use two model generated files, ENDPTS.ASC for trajectories and MDLCON.BIN for concentrations, to generate a Tektronix 4010 format output file called PLT.DAT. You may display and print this file with any compatible software or the HYTEK emulator that is provided with the model.

G.3 File Formats

A summary of all model generated files and a brief description of the format and contents follows:

ENDPTS.ASC - Particle endpoint positions for user applications or model restarting option. ASCII file with record length of 70 bytes.

Format	Field
I2	Year
I2	Month
I2	Day
I2	Hour
F6.2	Latitude (deg)
F7.2	Longitude (deg)
I5	X-grid position
I5	Y-grid position
I5	Pressure height (mb)
I5	Vertical Index
I5	Particle Age (hrs)
I5	Particle depth (m)
I5	Sequential particle index
E14.6	Particle mass

ENDPTS.CFG - ASCII file with the label and grid information required for post-processing of trajectory images.

Record	Format	Field
1	Char	Directory in which ENDPTS.ASC resides
2	6I6	Maximum dimension of meteorological grid in I,J,K; Beginning month, day, and hour, of the calculation.
3	5F12.4	Meteorological grid description: size in km, true latitude, x-pole position, y-pole position, grid orientation longitude.

4	7F6.1	Output map parameters: interval for lat/lon lines, left and right longitudes, top and bottom latitudes, latitude and longitude of the source point.

MDLCON.BIN - Binary unformatted dump of concentration grid values for re-display of calculated concentration fields.

Format	Field
Integer-4	Sequential emission number
Integer-4	Year
Integer-4	Month
Integer-4	Day
Integer-4	Hour
Integer-4	Forecast Hour
Real-4	Gridded concentrations of sub-grid domain

MDLCON.CFG - ASCII file describing the label and grid information required to read the MDLCON.BIN file.

Record	Format	Field
1	Char	Directory in which MDLCON.BIN resides
2	5I6	Maximum dimension of concentration grid in I,J,K; output level index of grid, averaging time in hours.
3	5F12.4	Concentration grid description: size in km, true latitude, x-pole position, y-pole position, grid orientation longitude.
4	7F6.1	Output map parameters: interval for lat/lon lines, left and right longitudes, top and bottom latitudes, latitude and longitude of the source point.
5	12I6	Heights in meters above ground of each concentration grid plane. Maximum value defined as K index (3rd variab) in line 2.

MDLTEST.CFG - ASCII file, see Appendix F for description.

MDLTEST.DAT - ASCII file, see Appendix E for description.

METFILE.CFG - Contains the grid descriptors for a variety of different meteorological grids that are available. It is an ASCII file of record length 130 bytes.

Format	Field
A10	Meteorological grid label
I3	Grid identification number
I3	Lowest west-east grid coordinate
I3	Highest west-east grid coordinate
I3	Lowest south-north grid coordinate
I3	Highest south-north grid coordinate
2X,F6.1	Meteorological grid spacing (km)
F6.1	Grid spacing true at this latitude
F6.1	West-East grid coordinate of pole
F6.1	South-North grid coordinate of pole
F6.1	Longitude at which south-north grid aligned
12F6.4	Sigma level of each vertical plane from bottom

EZMPDAT - The map background file is in NCAR graphics format as a variable length, unformatted file. Each record contains the latitude/longitude pairs that make up one line.

Format	Field
Integer-4	Number of points to read (NPTS)
Integer-4	Line identification
Real-4	Biggest latitude along the line
Real-4	Smallest latitude along the line
Real-4	Biggest longitude along the line
Real-4	Smallest longitude along the line
Real-4	NPTS numbers, where the first and second values represent the first latitude/longitude pair. There are NPTS/2 points that make up the line.

ROUGLEN - The aerodynamic roughness length for each degree of latitude and longitude. On input it is remapped to the current meteorological grid. Each data value is a 2 byte integer in centimeters. There are 360 x 180 data values. Each record contains 360 values from -180 to +180 (west to east). There are 180 records that go from latitude +90 to -90. You may also have an optional file called *TERRAIN* on your disk which contains the terrain height in meters in the same format.

SITES.ASC - An input file for program GRID2STN listing the station names and their latitudes and longitudes. The concentrations at these locations will be interpolated from MDLCON.BIN.

Record	Format	Field
1	List	Concentration conversion factor used to multiply each value in MDLCON.BIN before it is output.
2	end List	Six character station name, Station latitude (deg.hundreds), Station longitude (deg.hundreds).

MDLCON.ASC - The ASCII output file from program GRID2STN giving the concentrations for the stations listed in SITES.ASC.

Format	Field
I3	Start time of sample average: year
I3	Month
I3	Day
I3	Hour
10F6.1	Concentrations at up to 10 stations

APPENDIX H - HYTEK Tektronix Terminal Emulator

The HY-SPLIT graphics post-processing programs produce an output file called PLT.DAT. The images in this file are represented in a Tektronix 4010 format. The images can be printed or displayed with any commercially available emulator. However, for convenience a simple emulator, HYTEK, is provided with the HY-SPLIT model. It is highly suggested that this program be run only on computers with a math co-processor. The emulator can be used to display or print the PLT.DAT file. Supported printers include EPSON type dot matrix and Hewlett Packard Laser Jet and Paint Jet printers. The key difference between HYTEK and other emulators is that the graphics image on the screen is not just dumped to the printer, which only provides a print resolution comparable to that of the screen, instead the image is simultaneously drawn in a reserved memory area at the same resolution as the standard 1024 x 1024 tektronix screen. It is this memory image that is dumped to the print device. HYTEK can also be used as a communications program at up to 2400 baud through the serial port. In this way the HY-SPLIT model and post-processing can be done on a remote computer and the image displayed locally.

H.1 First Time Installation

HYTEK.EXE can be installed on any directory set in the path. However, the configuration file (HYTEK.CFG) must reside in the local directory. The HY-SPLIT install batch file installs HYTEK in the GRAPHIC sub-directory since the post-processing is done there. If your computer setup matches the default setup in HYTEK.CFG then HYTEK will start properly and it is quite likely you can edit the CFG file from within HYTEK by invoking the Ctrl-X option. However, if you get any startup errors, usually rather cryptic messages with a numeric code, then you must first edit the CFG file using any standard ASCII file editor. There are three fields on each line within double quotes, separated by commas. Normally you would only edit the first field. The others are for information and used in HYTEK as prompts. The exception is the RGB color indices, which can be edited. Follow the instructions below regarding setting the options in the CFG file.

Error Trapping:

Turn off (OFF) extended error handling unless you are running on a 386 class PC as it slows down processing considerably. Turn it on (ON) during the initial installation. Then turn it off for subsequent routine operations.

Printer Type:

There are three types of printers that are supported -- HP Laserjet (LJ), HP Paintjet (PJ), and EPSON dot matrix (DM). The PJ option will provide support for 16 colors.

Dots per inch:

This parameter can be used to control the size of the printed output. Valid options are those that apply to your particular printer. Regardless of the dot density selected the quality of the printed output will be the same. The smallest plot is obtained with 300 dpi, the largest with 100 dpi. Options for the Paint Jet are only 90 and 180 dpi.

Color Planes:

Always choose (1) for black and white (B&W) printing. Select (4) for color printing. Selecting fewer color planes reduces the number of color choices available (2^planes). However, additional color planes require more memory and slow down the processing. Therefore, if you have memory restrictions on your PC it may be necessary to limit the color choices. Although you can do B&W with four color planes, it is best to limit it to one plane for B&W printers.

Screen Resolution:

Screen resolution (CGA/EGA/VGA) is independent of printer output resolution. The full Tektronix image is mapped into the current screen with whatever resolution is supported. However, the print image is mapped to memory at a one-to-one pixel resolution.

Monitor color options:

Only color (COL) or monochrome (MON) are available options. The selection of the color option only affects the display and not the printing.

Left, Right, Top, and Bottom boundaries (printport):

Due to memory limitations of 64KB per color plane, it is necessary to select a smaller print window of the full 1024 by 1024 Tektronix screen. Since the pixel mapping is one-to-one, eight pixels of the 1024 x 1024 screen can be represented by one byte. This means that only about a 700 x 700 area can be printed at any one time. However, any subregion can be selected and it need not be square. The numbering system, representing the horizontal and vertical pixel number of the 1024 screen, increases from left to right and from top to bottom.

Screen Scaling:

The selected print window may fill the screen in relative coordinates (REL) or be shown in its true position on the 1024 by 1024 display in absolute (ABS) coordinates. This option only affects the screen display and does not affect printing. The REL option means that the printport is mapped to fill the entire screen. Using the ABS option will result in the screen representing the full 1024 display and the printport will appear as a box in its respective position on the screen. The ABS option is most useful in trying to position the printport over an image. In the ABS option the image will always be drawn in its proper location even if the printport does not cover it.

Baud Rate:

If you are using this program for communications through the serial port then you can select either 300/1200/2400 baud rates. If no communications is selected this option has no effect. Note that slow computers may have buffer overrun problems. No handshaking protocols are supported.

Parity:

Only none (N), even (E), or odd (O), are supported.

Data Bits:

Only seven (7) or eight (8) are valid options.

Local Echo:

Do you want the commands that you type on the keyboard echoed on the screen (Y) or will your entries be repeated by the host computer, which in that case you will select (N).

Input COM port:

If you are using HYTEK as a terminal emulator then set this value to the COM port (either 1 or 2) to which your modem is connected. A math co-processor is almost mandatory to avoid buffer overflow. If you are reading a Tektronix data file, as might have been generated by HYSPLIT, set the port equal to 0, and communications will NOT be enabled.

Input Data File Name:

This is the default data file name that will be opened for input when COM=0. It is usually defaulted to PLT.DAT as generated by HY-SPLIT graphics output. However, any file that exists may be entered here. It must reside in the default directory and it must exist, otherwise an error message will be generated.

Printer Path:

Select COM if you have a serial printer connected to one of your com ports (the one other than what the modem is connected to) or select LPT if you have a parallel printer connection. If you don't know -- ask someone.

Printer Port:

Select the port number for either COM or LPT selected previously. Valid options are 0, 1, or 2. If you select "0" you are disabling the printer. If you print with the printer disabled, the program will open a file called PCL.101 and write the print image to that file. Subsequent print requests increment the file by one, ie PCL.102, PCL.103, etc. These files are binary images that can subsequently be printed at the DOS level through the command: copy /b pcl.101 prn.

Background Color:

The graphics background color index is selected by the color palette number listed in the following entries.

Color Selections:

There are sixteen lines of color definitions consisting of three fields each. The first field names the color and the second field associates

that color with an index or palette number. The third field defines the color for printing. The display or printing of color is done through an index number. For HY-SPLIT post-processing graphics the colors are defined and associated with an index in a file called KOLMAP.DAT. This previously defined index can be associated with any color in HYTEK through redefinition in this table. HYTEK can only be used to edit the first field. If you need to edit any of the others use a ASCII text editor. The only time you may want to edit the third field is if the colors that the Paint Jet printer produces require some adjustment for improved visual clarity. See the printer manual for instructions about the constants associated with each color.

H.2 Standard Operation after proper initialization

Upon first starting HYTEK a portion of memory is prepared for saving the graphics image, this initialization may take many minutes on XT class PCs to a few seconds on a 386 machine. After initialization an initialization file is written (ZERO.001 to .004 for each color plane) which is used if subsequent initializations are needed. A help menu is displayed next showing all the commands to which HYTEK responds. All HYTEK commands are preceded by the Ctrl key. Pressing any key will clear the help menu. The program then waits for another key press before continuing in file mode or communications mode. The HYTEK commands are summarized below:

Ctrl	Command Summary
B -	Sends break signal out the COM port when HYTEK is in communications mode.
C -	Clears the graphic display and memory image. When background mode is enabled (see Ctrl-S) it resets the initialization back to the ZERO.00X file.
E -	Exit the emulator.
F -	Input/Output file toggle. Opens and closes new files for I/O. In file mode it is used to specify a new input file when, for instance, you have finished displaying the image in PLT.DAT, or the image you want to display is in a different file than the one defined in the CFG file. In communications mode it defines an output file in which the incoming Tektronix data can be captured. The capture file name defaults to TEK.101 with subsequent increments in the suffix for each invocation of Ctrl-F.
G -	Autoprint toggle on/off. Works best in file mode when you have multiple frames on one file. When the toggle is set to on the displayed image will be sent to the print device if no command is entered for 10 seconds after the image drawing is completed. The print device can be set to LPT=0 so that a new output file PCL.10X is created with each image. To work properly it is necessary to invoke the command before the first image is drawn. The last

image in a file will not be printed unless the file was created with an additional frame at the end. This frame can be blank, as all HYTEK needs is the new frame command to trigger the printing.

H - Backspace for communications mode.

K - Color select toggle. Each press of the key will result in the color index to be incremented by one. This can be used to override color palette commands in the file or to generate a color image from a black and white file.

L - Loads graphics image to memory. A map background, or any image can be saved on a disk file (see Ctrl-S) so that when a new image is drawn it will be drawn on top of this image. This command will load that image from a file called BKGD.00X each time it is invoked. When a new frame is started the BKGD file is automatically loaded into memory, rather than the ZERO file, to initialize the graphics image. This can be cleared back to a blank image by pressing Ctrl-C.

P - Prints the internal graphics image to the current print device. This device can be defined as either LPT or COM 0/1/2 in the CFG file. A definition of "0" disables printing to a device and instead sends the print image to a file called PCL.101. This file can be printed later on the DOS level by the command: copy /b pcl.101 prn. Each invocation of the command increments the file suffix by one.

R - Read and skip the next frame. On multi-frame inputs HYTEK will only read the next graphics frame and not display or interpret it. It will pause at the next new frame character. This method is slightly faster than displaying unwanted graphics images.

S - Saves the current internal graphics image to a file (BKGD) and sets an internal toggle so that when a new graphics frame is started this image will be loaded rather than the blank map image (ZERO).

X - Invokes the HYTEK configuration (CFG) file editor, which permits modification of any of the first field parameters. Exiting from this will result in reinitialization of the graphics memory printport.

Z - Redisplay of the help menu.

H.3 Command Line Operation

Normally HYTEK is called from the DOS command line and after initialization it will wait for appropriate user prompts. However, sometimes it is desirable to use the emulator in a batch file to convert or print multiple graphics frames without operator intervention. This automatic

process is invoked on the command line by following HYTEK with a FILENAME. The program will then process that file according to the current configuration in HYTEK.CFG. Options can be set to print frame in the file or convert each frame to a printable PCL file.

APPENDIX I - HY-SPLIT ERROR CODES

Certain conditions will trigger premature termination of the HY-SPLIT model simulation. If the simulation is performed in a non-graphics environment the messages will appear on the display. If the graphics output option is selected, error messages will be written to a file called HYSPLIT.MSG in the output directory. A summary of how these error codes can be interpreted follows:

Code	Description
	METINPUT
101	There was an error in reading the header label information at the beginning of a meteorological data record in the meteorological data input subroutine. Normally this error would not occur during the initial execution as the data are checked by several other routines first. However, if the data became garbled further in the file it would be caught in the normal input routine. Another possibility is that you reached the end-of-file and requested a new file to continue calculations and this new file is not in the correct format or is from a different data grid. Subsequent file opens do not undergo extensive testing.
102	In the normal opening sequence the model can't position itself in the meteorological data file within two attempts to the correct starting record to match the requested start time. This can occur if there are extensive missing or duplicate data records in the meteorological file near the time that the model is trying to position itself. Another possibility is that there are multiple months of data on the file. The model can only handle a maximum of two months per file. One solution might be to break-up the file into smaller data groups. Missing or duplicate data problems can be edited with the meteorological data file utility program--GAMDUP.
103	Similar to 102 except after positioning the time in the header of the record doesn't match the requested time.
104	There was an error in interpreting the header label of the meteorological data record in the initial meteorological data file evaluation program. This error is most likely due to specifying the wrong grid dimensions, in x and y, for the data file requested. These dimensions are set in METFILE.CFG. The possible reason for this occurring is that you are using an old meteorological data set created before the grid ID numbers were standardized, resulting in the model matching the meteo file grid ID with a similar ID in the METFILE.CFG that identifies the wrong data grid.

105 The model can't find the METFILE.CFG file. The usual reason for this and similar "can't find errors" is that the directory for input data files in DEFAULT.CFG points to the wrong directory.

106 In this situation the grid ID written in the header label of the meteorological data record can't be matched with any ID number found in METFILE.CFG. Presumably you just got a new data file to run but you forgot to update the METFILE.CFG to reflect the additional data.

107 The DEFAULT.CFG file permits you to select a variety of sub-grids. For instance few PC models have sufficient memory to read in the entire 65 x 65 northern hemisphere MRF data archive. Normally the model will default to a subset of the data grid that matches the dimensions for which the code was compiled. However, the default sets the lower left corner at grid point 1,1. You may not want to simulate only the South Pacific, therefore you can define your meteorological data sub-grid anywhere over the domain as long as the delta-x and delta-y of your sub-grid do not exceed the compiled dimensions. If they do you must either alter the sub-grid or recompile if the larger domain is required.

108 The routine that sets the model grid characteristics cannot read the header record of the meteorological data file. This is the first time that the meteorological data are read by the model, so that the error at this point suggests that even the first data record is garbled. Perhaps there was an inadvertent ASCII to EBCIDIC conversion.

109 A model report that southern hemisphere data is not available can mean several things. First it is looking for southern hemisphere data because you requested a starting latitude that was negative. Therefore, the initial file that is opened must be identified in METFILE.CFG as a file that has a grid with a true latitude of less than zero. If that is not the case the model next assumes that the southern hemisphere data must be concatenated to the northern hemisphere data. Typical, although not required, in the archive format is that each data time contains the northern hemisphere data followed by the southern hemisphere data. If this is not the case then the model assumes we are looking at a forecast format (not discussed in Appendix D) in which the southern hemisphere forecast data follows the northern hemisphere data after the last forecast field (72 h). If none of these conditions are met then the error message will be displayed. Note that although the northern hemisphere data sets extend into the southern hemisphere it is not possible to start a trajectory in the other hemisphere for either hemisphere's data. The only way to bypass this restriction is to create an ENDPTS.ASC file that contains the starting point and let the model continue the calculation from that point.

401 Model can't find the DEFAULT.DAT file. Check to make sure that the input file directory is properly set in DEFAULT.CFG.

402 The model looks for DEFAULT.CFG in the home (default) directory. The model needs to read this file before it knows in what directory the other files are located. The HY-SPLIT batch file first copies the DEFAULT.CFG file from the CFGFILE sub-directory to the EXECMDL sub-directory. If you get this error you are probably running the model directly rather than through the batch file.

403 The file MDLCON.BIN is only required when you are going to be appending to it. As it is primarily an output file, even when used for input it is defined in the output files directory in DEFAULT.CFG.

404 The ROUGLEN.BIN file contains a global extract of the aerodynamic roughness length. It is required to be in the input files directory.

405 The ENDPTS.ASC can be used for input or output. Depending upon its usage as defined in DEFAULT.DAT it must reside in the appropriate input or output directories as defined in DEFAULT.CFG.

EMISSION

701 It is possible to define the latitude and longitude of a source point off the meteorological data grid. This message appears when that condition occurs. The message also contains the coordinates that should be entered in DEFAULT.CFG for the lower left corners (in x and y) of the meteorological sub-grid so that the selected origin lies in the center of the meteo sub-grid.

GRAPHICS

801 The model cannot set the graphics mode for any number of reasons such as an unsupported video graphics mode. The only solution to this is to turn off the run-time graphics option in DEFAULT.DAT.

802 The run-time graphics setup program cannot find the scalable font file: MODERN.FON. It should be in the input files directory. Another possibility is that the file became corrupted. If you have Microsoft fortran available just copy the font file from that directory to the HY-SPLIT CFGFILE sub-directory.

803 The run-time graphics setup program cannot set the font size for a number of unknown reasons. Turn off run-time graphics. Another possibility is that there is some interference from a TSR program. Try re-bootting first before trying to remove some resident programs.

804 There was an error in reading data from the map background file EZMPDAT. Perhaps the data has been corrupted and it is necessary to obtain a replacement.

APPENDIX J - VERIFICATION STUDIES

J.1 ANATEX Validation

The Across North America Tracer Experiment (see Draxler et al., 1991) was used to test the concentration calculation portion of the HY-SPLIT code. The results reported here are only a coarse summary of all the possible tests that could be performed. ANATEX consisted of 66 tracer releases evenly divided between two locations for a three month period during the winter of 1987. Sampling was conducted at distances of 100's to 3000 km from the tracer release points.

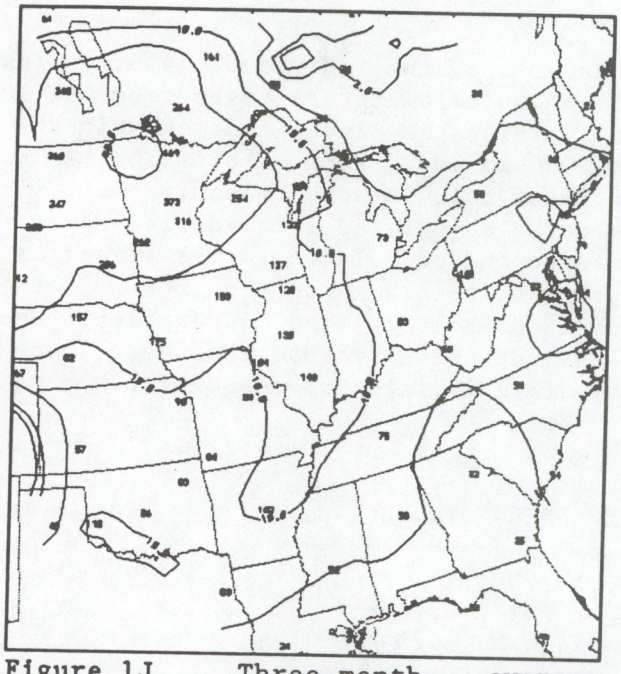


Figure 1J. Three-month average measured concentration for releases from both Glasgow and St. Cloud.

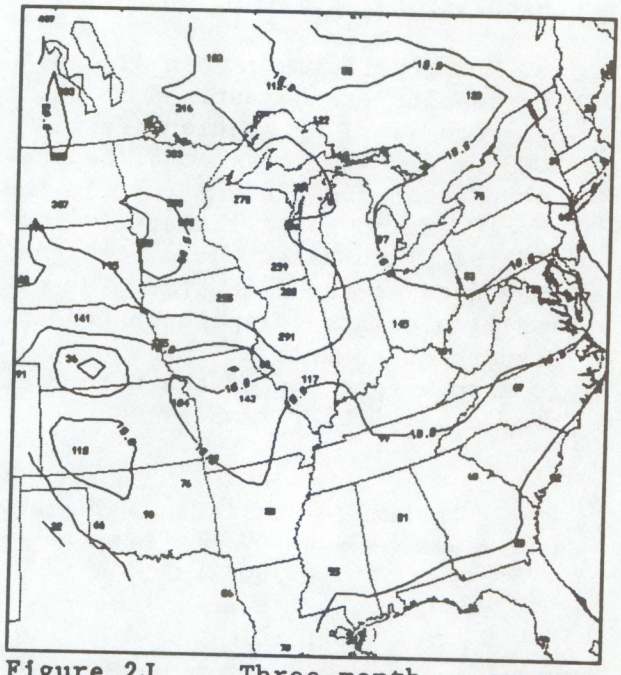


Figure 2J. Three-month average calculated concentration for release from Glasgow and St. Cloud.

The average tracer concentration expressed as the sum from both release locations (GGW-Glasgow, MT and STC-St. Cloud, MN) measured at the 77 sampling locations is shown in Fig. 1J. The measured data consists of a three-month time series of 24 h average concentrations. These were averaged at each site and shown in units of concentration by volume (parts in 10^{17}). Contours are drawn at about factor of two intervals (1, 2, 5, 10,...) at parts in 10^{16}. Note how the measured concentration only drops about a factor of ten from the source region, the north central states, to the Atlantic and Gulf coasts, the edge of the sampling domain.

The comparable model calculation is shown in Fig. 2J. This model simulation used only the first 6 sigma levels of the NGM meteorological data. In general the magnitudes of the calculations are similar to the measurements with the exception of some consistent over-prediction near the St. Cloud source region. The near-source over-prediction is due to a constraint within the model that forces the concentration summation routine to sum to at least one grid point each advection step. This eliminates the possibility that a narrow plume may slip through a coarser concentration sampling grid. The model prediction may be modified in this situation by increasing the concentration grid resolution until the model calculation is no longer sensitive to grid size. At further downwind distances the model calculation is quite good, also showing about an order of magnitude drop across the calculational domain.

Model performance can also be evaluated from the individual 24 h samples. The results are summarized in the table shown below for releases from GGW and STC with sampling stations sorted into two distance bands, those within the 2000 km arc and those at or beyond the 2000 km arc. Each combination has the correlation coefficient (corr), the ratio of calculated to measured concentration for all cases (mean) including calculated and measured zeros, and the plume cases where both the measured and calculated values were greater than zero at the same time. The plume statistic is a measure of how well the model calculates dispersion for an individual release. The mean reflects the dispersion as well as the accuracy of the advection because the overall mean is also a function of the number of times a calculated or measured plume was over a particular sampler.

Table 1.--Statistical summary of ANATEX simulations

	< 2000 km			>= 2000 km		
	corr coef	mean C/M	plume C/M	corr coef	mean C/M	plume C/M
GGW	.69	2.9	3.2	.32	1.4	1.8
STC	.34	1.7	1.7	.11	1.6	1.5

For unkown reasons, calculations at GGW are much better than at STC as represented by the correlation. However, GGW releases show much more over-prediction than STC releases at the close-in samplers. The three samplers surrounding STC were excluded from the calculations. The causes are difficult to evaluate; one possibility is that because the close-in samplers around STC surround the release site, while the GGW samplers are at least 500-km distant, and in a sector that requires West or North-West winds, results in difficult synoptic regimes being under-represented in the GGW releases while STC releases would sample all types of synoptic events. Perhaps the W-NW flow associated with GGW releases has much more dispersion than estimated by the model.

J.2 CAPTEX Validation

The CAPTEX experiment was conducted during September and October of 1983 consisting of four perfluorocarbon releases from Dayton, Ohio and two from Sudbury, Ontario. Six consecutive samples were collected at 84 locations for each tracer release. Sample durations varied from 3 to 6 hours depending upon distance from the release site. In contrast to ANATEX, tracer releases only occurred when the tracer plume was forecast to go over the sampling network.

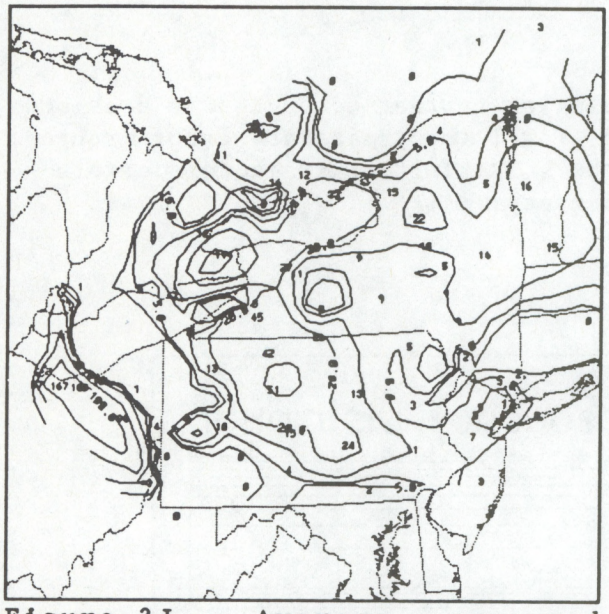


Figure 3J. Average measured concentration (fL/L) from all CAPTEX releases.

Figure 4J. Average calculated concentration from all the CAPTEX tracer releases.

Model simulations of the CAPTEX experiment are a little different in that no NGM data are available for this period. Rawinsonde observations were used in conjunction with the gridding program *WT2GRID* to produce a model readable input file from which concentration calculations were made. A plot of the average measured concentration for all releases, similar to the ANATEX results, is shown in Fig. 3J and the comparable model prediction is shown in Fig. 4J. Due to the higher background of the tracer used in CAPTEX to that in ANATEX, concentration values are an order of magnitude higher. The plotted values and contours are shown in volume units of tracer in 10^{15} units of air.

The resulting measured and calculated concentration patterns are more complex than the 3-month ANATEX averages due to the limited number of releases. In general model calculations are somewhat less than the measurements. One particular, interesting feature is the measured concentration "gap" just east of the Dayton release site. Model calcualations show a much more gradual concentration decrease. Presumably this is due to the decoupling of the tracer plume from due ground during the night. As all Dayton releases started in the early afternoon, the Ohio-Pennsylvania border region would correspond to the approximate tracer position at the beginning of the evening.

The statistical summary in the table below, similar to that made for ANATEX, shows that the correlation is comparable, while the mean concentrations are under-calculated. Plume calculations are comparable to the measurements.

corr coef	mean C/M	plume C/M
.36	.84	.99

In an analysis of trajectory error, similar to that conducted in previous CAPTEX simulations, showed that after 24h travel the trajectory errors ranged between 0.20 to 0.30 of the travel distance. The initial trajectory errors ranged from 0.25 to 0.35 of the travel distance.

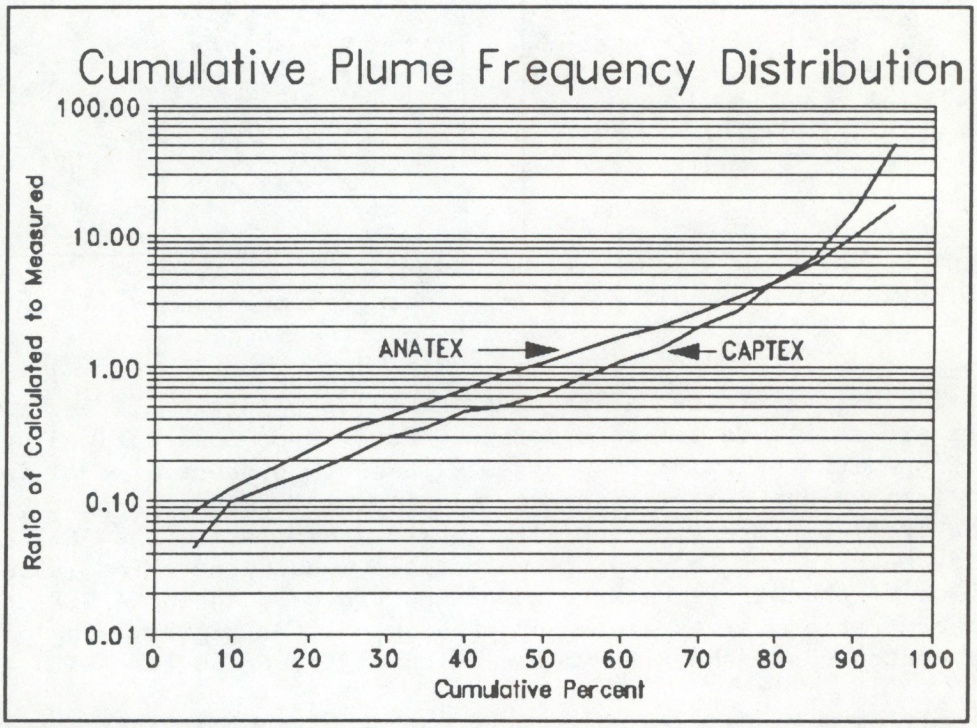


Figure 5J. The ratio of calculated to measured concentration pairs sorted by cumulative percent for the CAPTEX and ANATEX experiments.

J.3 CAPTEX versus ANATEX

Although there are considerable differences between the two experiments, one simple comparision would be how well the model predicts the plume dispersion. Those cases when both the measured and calculated concentration is greater than zero. To make the CAPTEX data more comparable to ANATEX the concentrations at each sampling location were averaged over each experiment, resulting in an 18 to 36 h average concentration, comparable to the ANATEX 24 h sampling periods. The resulting individual calcualated to measured concentration ratios were then sorted and are shown as a cumulative frequency distribution in Fig. 5J.

Overall the two distributions are remarkably similar, with CAPTEX showing a median ratio of 0.6 and an ANATEX median closer to 1.0. Fifty percent of the CAPTEX predictions range over an order of magnitude (0.2 to 2.0) while 50% of the ANATEX calculations also range over an order of magnitude (0.3 to 3.0).

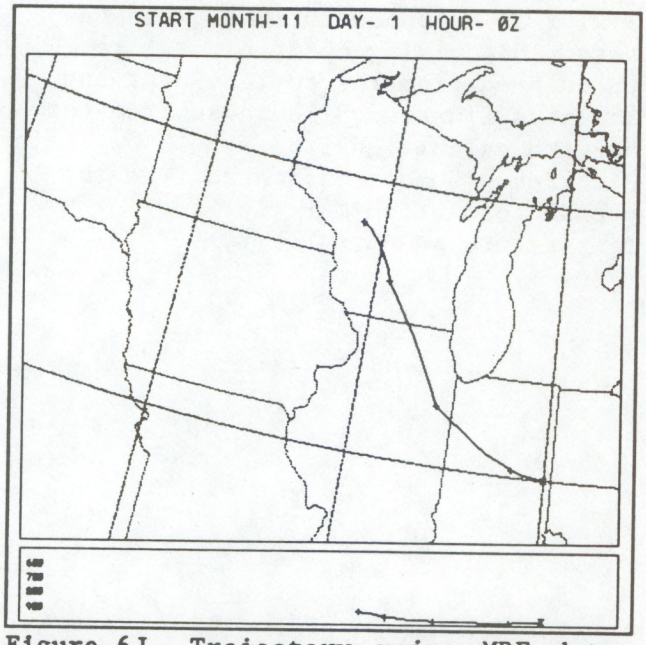


Figure 6J. Trajectory using MRF data, comparable to the case shown with NGM data in simulation test005.

Meteorologically the main difference between the two experiments is that CAPTEX was a summer experiment while ANATEX was conducted in the winter. The differences in model performance between summer and winter suggests that the calculated mixing is probably too little in winter and too great in summer. Improved model predications can probably be achieved by reducing the range of calculated vertical mixing. With the current model mixing parameterization, this is difficult to accomplish, without a major revision of how that part of the model is designed.

J.4 NGM versus MRF calculations

Although comparing calculations with NGM and MRF data is not a validation, it provides an additional measure of uncertainty that can be expected from these type of calculations. As a special test meteorological data for the same period (Nov. 1, 1991) were extracted for a sub-grid over the continental U.S. from the MRF archive. The MRF trajectory for the same case (test005 - Fig. 8) that was shown in the main text is illustrated in Fig. 6J. Note that it is somewhat slower than the NGM trajectory and hence intercepts the low (where the cyclonic curvature begins) further to the east. Further the vertical motion associated with the low also drives the trajectory upward as it moves west.

A similar comparison can be made for the air concentration calculations. In that case the NGM simulation test006 (Fig. 10) is rerun with the MRF data and is shown here in Fig. 7J. The range of concentrations and maximum values are similar, although not identical. This is to be expected due to differences in the trajectory, wind speed, and of course how the vertical mixing is computed for the two data sets. NGM mixing coefficients are calculated from the surface heat and momentum fluxes, while those from the MRF are calculated from a bulk Richardson number estimated from the coarse resolution MRF wind and temperature sounding.

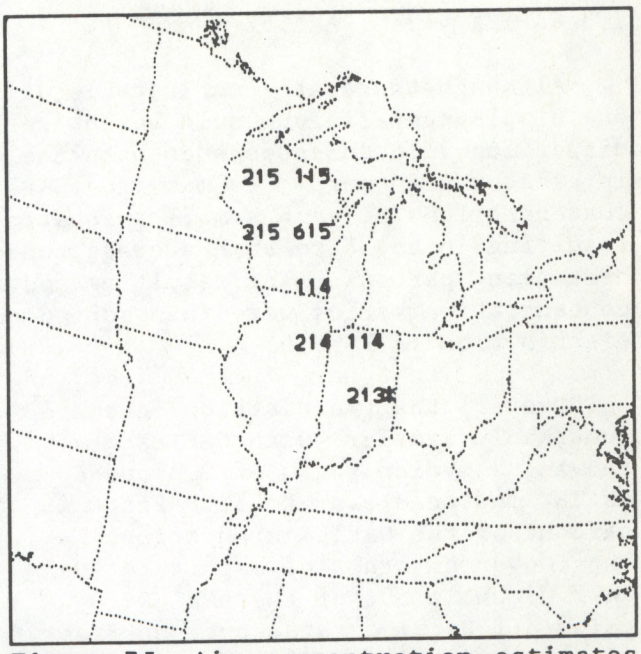


Figure 7J. Air concentration estimates using MRF data, similar to the NGM case shown in Fig. 10 (test006).

U.S. GOVERNEMNT PRINTING OFFICE: 1992-673-025/69009