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HYSPLIT_4 USER's GUIDE

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INFORMATION

This document discusses the technical aspects of the installation and operation of the Hysplit4 model version designed to run on Windows 95/98/NT platforms. The code can be obtained at: http://www.arl.noaa.gov/hysplit.html.

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HYSPLIT 4 USER'S GUIDE

ABSTRACT. The HYSPLIT_4 (Hybrid Single-Particle Lagrangian Integrated Trajectory) Model installation, configuration, and operating procedures are reviewed. Examples are given for setting up the model for trajectory and concentration simulations, graphical displays, and creating publication quality illustrations. Programs that can be used to create the model's meteorological input data are described.

1. MODEL OVERVIEW

1.1 Features

The HYsplit_4 (HYbrid Single-Particle Lagrangian Integrated Trajectory) model is a complete system for computing trajectories to complex dispersion and deposition simulations using either puff or particle approaches.¹ It consists of a modular library structure with main programs for each application: trajectories and air concentrations.

Gridded meteorological data, on one of three conformal (Polar, Lambert, Mercator) map projections, are required at regular time intervals. The input data are interpolated to an internal sub-grid to reduce memory requirements and increase computational speed. Calculations may be performed simultaneously on multiple meteorological grids, from fine to coarse resolution.

Air concentration calculations require the definition of the pollutant's emissions and physical characteristics. When multiple pollutant species are defined, an emission would consist of one particle or puff associated with each pollutant type. Alternately, the mass associated with a single puff may contain several species. The latter approach is used for calculation of chemical transformations when all the species follow the same transport pathway. Chemical transformation subroutines are not part of the model distribution.

The dispersion of a pollutant is calculated by assuming either a Gaussian or Top-Hat horizontal distribution within a puff or from the dispersal of a fixed number of particles. A single released puff will expand until its size exceeds the meteorological grid cell spacing and then it will split into several puffs. An alternate approach combines both puff and particle methods by assuming a puff distribution in the horizontal and particle dispersion in the vertical direction. The resulting calculation may be started with a single particle. As its horizontal distribution expands beyond the grid length scale, it will split into multiple particle-puffs, each with their respective fraction of the pollutant mass. In this way, the greater accuracy of the vertical dispersion parameterization of the particle model is combined with the advantage of having an expanding

¹Draxler, R.R., and G.D. Hess, 1998, An overview of the Hysplit_4 modelling system for trajectories, dispersion, and deposition, Australian Meteorological Magazine, 47, 295-308.

number of particles represent the pollutant distribution as the spatial coverage of the pollutant increases.

Air concentrations are calculated at a specific grid point for puffs and as cell-average concentrations for particles. A concentration grid is defined by latitude-longitude intersections. Simultaneous multiple grids with different horizontal resolutions and temporal averaging periods can be defined for each simulation. Each pollutant species is summed independently on each grid.

The routine meteorological data fields required for the calculations may be obtained from existing archives or from forecast model outputs already formatted for input to Hysplit. In addition, pre-processor programs are provided to convert NOAA, NCAR (National Center for Atmospheric Research) re-analysis, or ECMWF (European Centre for Medium-range Weather Forecasts) model output fields to a format compatible for direct input to the model. The model's meteorological data set structure is compressed and in "direct-access" format. Each time period within the data file contains an index record that includes grid definitions to locate the spatial domain, check-sums for each record to ensure data integrity, variable identification, and level information. These data files require no conversion between computing platforms.

The modeling system includes a Graphical User Interface (GUI) to set up a trajectory, air concentration, or deposition simulation. The post-processing part of the model package incorporates routines for simple screen displays of air concentrations and trajectories as well as more sophisticated graphical programs to generate multi-color or black and white publication quality Postscript printer graphics.

A complete description of all the equations and model calculation methods for trajectories and air concentrations has been published,² and is also available on-line (http://www.arl.noaa.gov/hysplit.html).

1.2 Pre-Installation Preparation

Although the self-installing executable, hysplit4.exe, does not require any additional software, it will only provide a command line interface to the model. To enable the model's GUI, the computer should have Tcl/Tk script language installed. It can be obtained over the Internet from: http://www.scriptics.com, or ftp://ftp.scriptics.com. The installation of Tcl/Tk will result in the association of the .tcl suffix with the Wish executable and all Hysplit GUI scripts will then show the Tk icon.

The Hysplit GUI contains options to convert either the trajectory or concentration model output files to Postscript. The Postscript files can also be viewed directly through the GUI if a

²Draxler, R.R., and G.D. Hess, 1997, Description of the Hysplit_4 modeling system, NOAA Technical Memorandum ERL ARL-224, December, 24p.

Postscript viewer, such as Ghostscript has been installed prior to the Hysplit installation. See www.cs.wisc.edu/~ghost for more information on Postscript viewers.

1.3 Windows 95/98/NT Installation

Hysplit installation to a computer running Windows (16 bit versions are not supported) is provided through a self installing file. Executables are provided in various directories for trajectories, dispersion, display of results, manipulation of results, and creation of input meteorological data files. The trajectory and dispersion model source code is not provided. However all the Fortran source code to create meteorological data files in a format that the model can read are provided in the \metdata directory. Each subdirectory contains a *Readme.txt* file with more complete information about the contents of that directory.

At the beginning of the installation you will be prompted as to the directory location. It is suggested you select the default location (C:\hysplit4). The installation program is very simple and although the selection of a different drive or directory will install the code in the selected directories, the shortcut links will not be placed correctly in the Start Menu or Desktop. In this situation you will need to edit the \icons\setup.bat file for the correct drive and directory locations.

The following subdirectories will be created after the installation has completed:

bdyfiles - This directory contains an ASCII version of gridded land use and roughness length data. The current file resolution is 360 x 180 at 1 degree. The upper left corner starts at 180 W, 90 N. The files are read by both Hysplit executables, hymodelt and hymodelc, from this directory. If not found, the model uses default constant values for land-use and roughness length. The data structure of these files is defined in ASCDATA. CFG, which should be located in either the model's startup directory or the \bdyfiles directory. This file defines the grid system and gives an optional directory location for the land-use and roughness length files. These files may be replaced by higher resolution customized user-created files. More information on the structure of these files can be found in the local Readme.txt file. Regardless of their resolution, the model will only apply the data at the same resolution as the input meteorological data grid.

data2arl - Current forecast or archive meteorological data can be obtained from the ARL ftp server: ftp://gus.arlhq.noaa.gov /pub/archives (or /forecasts). Older archive data can be ordered from the NCDC (National Climatic Data Center). However if you have access to your own meteorological data or data formatted as GRIB (Gridded Binary), this directory contains various example decoder programs to convert meteorological data in various formats to the format (ARL packed) that Hysplit can read. Sample programs include GRIB decoders for ECMWF model fields, NCAR/NCEP (National Centers for Environmental Prection) re-analysis data, and NOAA Aviation and Regional Spectral Model files. All the required packing and unpacking subroutines can be found in the \source sub-directory. More information on these programs can be found in Section 5.4.

concmdl - The directory contains the Hysplit4 air concentration prediction model (hymodelc) and related display programs. Although the model can be run through the GUI, at times it may be desirable to run the model from the command line (e.g. using automated scripts). The example Control file should produce some results for viewing. The sequence of commands would be hymodelc to execute the model, wincplot to display the graphical output, and concplot to create a Postscript file called concplot.ps. Command line arguments are required for concplot. Normally the GUI is used to create the Control file for the simulation. If the file is missing, the model will prompt you for input from the keyboard. Your inputs are copied to a file called Startup. That file may then be edited and renamed to Control for subsequent simulations. Conread and con2asc are provided as examples of how to read concentration files for user applications.

document - This directory contains PDF (Adobe Portable Document Format) versions of the User's Guide and other documentation such as ARL-224, the principal ARL Technical Memorandum describing the model and equations. This User's Guide (this document) provides detailed instructions in setting up the model, modifications to the *Control* file to perform various simulations and output interpretation. The *Readme.txt* file contains additional information about compilation, typical CPU times, and a summary of recent model updates.

graphics - There are two types of graphical plotting programs provided in the \concmdl and \trajmdl directories. The screen display programs, wintplot and wincplot, use the Microsoft Fortran QuickWin graphics library. However printed resolution is limited to the screen's resolution. Publication quality graphics can be created using the postscript conversion programs, concplot and trajplot, which use a Fortran Postscript library created by Kevin Kohler³. All graphical routines use the map background file arlmap in this directory. The map background file uses a simple ASCII format and contains the world's coastal and political boundaries at relatively coarse resolution. Other higher resolution map background files are available from the Hysplit download web page. All graphical programs search the startup directory first for arlmap before going to \graphics, therefore customized maps can be created without changing the Hysplit installation structure.

guicode - This directory contains a Tcl/Tk GUI interface source code script for Hysplit. The interface is used to set up the input Control file as well as run the graphical output display programs. To use the interface you must first install Tcl/Tk. The upper-level Tcl script is called hysplit4.tcl, which calls all other Tcl scripts. The Hysplit GUI is started by executing this script. The Desktop short-cut as well as the Start Menu options should point to this script. If the installation program did not properly setup the Desktop, you should copy the shortcut from \working or you can manually create a short-cut to the script and edit its properties such that the "Start In" directory is \working. You should also select the Hysplit icon from the \icons directory before moving it to the Desktop.

³PSPLOT libraries can be found at www.nova.edu/ocean/psplot.html and were created by Kevin Kohler (kevin@ocean.nova.edu).

icons - Normally if you install Hysplit to the default drive c:\hysplit4, there should be a desktop icon as well as entries in the Start Programs menu. If these short-cuts were not set up properly, you can edit the Setup.bat file to reflect your directory structure. If you still have trouble, then the icons supplied in this directory can be used to replace the default Windows icons if you create shortcuts to Hysplit from the desktop. Use the right mouse button and select: Properties | Shortcut | Change Icon. Note that the \working\hysplit4.tcl shortcut should be copied to the desktop.

metdata - This directory contains the sample meteorological data file: oct1618.BIN. It is an extract of the NGM over the US from 0000 UTC 10/16/95 through 0000 UTC of 10/18/95. The file is used for all calculations shown in the User's Guide. In addition, several sample programs are provided that can be used to examine and display the meteorological data files. Source code for these routines can be found in the \source subdirectory. More information on these programs can be found in Section 5.4.

trajmdl - This directory contains the Hysplit4 trajectory model (hymodelt) and related display programs. Although the model can be run through the GUI, at times it may be desirable to run the model from the command line (e.g. automated scripts). The example Control file should produce some results for viewing. The sequence of commands would be hymodelt to execute the model, wintplot to display the graphical output, and trajplot to create a Postscript file called trajplot.ps. Normally the GUI is used to create the Control file for the simulation. If the file is missing, the model will prompt you for input from the keyboard. Your inputs are copied to a file called Startup. That file may then be edited and renamed to Control for subsequent simulations.

working - This should be the default working directory when running the model through the GUI. The properties of the Hysplit4 shortcut should point to this as the startup directory. This directory will contain all the user created input and output files unless they are explicitly directed to be read or written from/to another directory in the input Control file, such as meteorological data files that might be found in \methata. A sample tcl script, \textit{Auto_traj.tcl}, is provided as an example of how one might automate multiple trajectory calculations. The script creates the \textit{Control} file and executes the model in a loop, varying specific parameters with each simulation.

1.4 Quick Start

The easiest way to run the model is to use the GUI menu to edit the model's input *Control* file. For the purposes of this demonstration appropriate meteorological files are provided. If for some reason the menu system is not available, the *Control* file can be created manually. See the discussion in Section 2.

Step 1 - start the GUI menu system using \working\hysplit4.tcl or the desktop shortcut to Hysplit4. A widget will appear with the HYSPLIT graphic and two button options: Menu and Exit. On some systems the graphic may be scrambled or the colors may be flat. Switching the PC display to VGA and 256 colors usually solves these problems. However it can be left alone as the faulty graphic will not affect any of the other widgets or display graphics.

Step 2 - from the HYSPLIT graphic widget click on Menu. The three main menus of Hysplit4 will appear: Data FTP from ARL, Trajectory, and Concentration. An additional small widget underneath the main menu gives the current Hysplit4 version information. Do not delete this widget as it will terminate the GUI. It provides the frame for the model's standard output and messages.

Step 3 - for the first example calculation select the *Trajectory* option. Four options appear under this item: *Trajectory Setup*, *Run Model*, *Trajectory Display*, and *Convert to Postscript*. Normally these are run in sequence, however any item can be selected and run if the appropriate input files were created during a previous simulation.

Step 4 - Trajectory Setup is used to enter the basic model simulation parameters: the starting time of the calculation; starting location in terms of latitude, longitude, and height; the run-time or duration of the trajectory calculation; and the names and locations of all required files. Specified directory paths should always terminate with "\". When modifications to this menu are complete, click on Save. However for this example, you will use the Retrieve option for predefined configurations, so do nothing here and go on to Step 5.

Step 5 - for the sample calculation click on *Retrieve*, enter name of the example pre-configured control file: *sample_traj*, then click on *OK*, then after the data entry widget is closed, click on *Save* and the setup menu will close.

Step 6 - Run Model copies the setup configuration to the model's input Control file and starts the model calculation. Messages will appear on standard output showing the progress of the calculation. When the simulation is completed, the trajectory end-points output file is ready to be converted to a graphical display. Under Windows the standard output widget will not open until the end of the calculation, however all the Trajectory menu items will be locked until the calculation completes.

Step 7 - selecting *Trajectory Display* will run a special display program that converts the ASCII file of trajectory end-point positions for display on the computer screen. The windows display is automatically invoked. If everything has worked correctly, the sample control file and data will have produced a trajectory plot identical to the one shown in Fig. 1. The horizontal solid line represents the trajectory at elevation, while the green vertical lines project the trajectory position down to the ground marked with blue dots at 3-h intervals. The starting position is

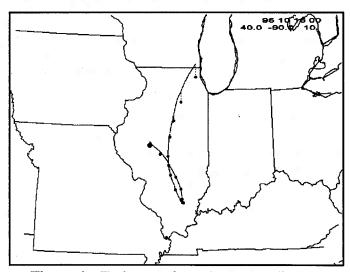


Figure 1. Trajectory from the screen display.

shown in red. The display may be printed or it may be copied to the clipboard and pasted into another application.

Step 8 - selecting Convert to Postscript will run a special program that converts the ASCII file of trajectory end-point positions into a high quality Postscript (trajplot.ps) suitable for printing. No messages appear during the conversion. However if a **Postscript** viewer (Ghostscript / Ghostview) has been installed and associated with .ps files, then it will be automatically invoked by the GUI. If the viewer does not automatically open, it may be necessary to manually edit \guicode\hysplit4.tcl to change directory location associated with the program gsview32.exe. The sample output from the Postscript file is shown in Fig. 2. Trajectory positions are marked at 6-h intervals and the vertical projection is shown in the lower panel.

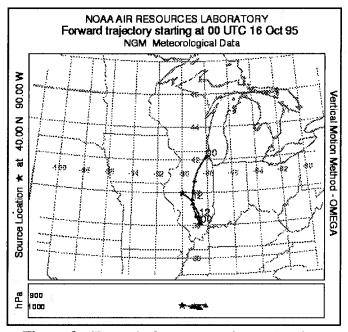


Figure 2. Example from Postscript conversion.

Step 9 - for the second example calculation select *Concentration*. Under this menu there are five options: concentration setup, run model, concentration display, convert to postscript, and convert to ascii. In general they should be executed in sequential order.

Step 10 - selecting Concentration Setup brings up similar starting information as with trajectories, but with three additional sub-menus (Pollutant) that can be used set the emission rate, duration, and start time of the emission; (Grids) to set the location, resolution, levels, and averaging times of the concentration output grid; and (Deposition) to set the characteristics of each pollutant. Click on Retrieve, enter name of sample pre-configured control file: sample_conc, then click on OK, then after the data entry widget is closed, click on Save and the setup menu will close.

Step 11 - selecting *Run Model* copies the setup configuration to the model's input *Control* file and starts the model calculation. Messages will appear on standard output showing the progress of the calculation after the calculation has completed. At that point the binary gridded concentration output file is ready to be converted to a graphical display. Be patient as concentration calculations may take considerably longer than trajectory calculations.

Step 12 - selecting Concentration Display directly plots the binary concentration file on a map background. The concentration pattern, color coded for each order-ofmagnitude range will be drawn directly to a window. If everything has worked correctly, the sample Control file and data will produce four different concentration maps, with the last pattern similar to the one shown in Fig. 3, which represents the last 12-hour averaging period of the 48-hour simulation. display can be printed or copied to the clipboard. The print quality is limited by the screen display. Note that the color filled boxes are the same size as the

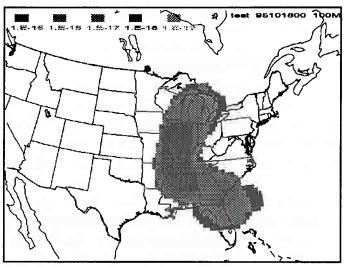


Figure 3. Concentration from the screen display.

resolution set for the concentration output grid. If the boxes are too large for a particular application, then the resolution must be reduced. See further discussion about the *Control* file in Section 2.2.3.

Step 13 - selecting Convert to Postscript will run a special program that converts the binary concentration file to a Postscript file (concplot.ps) suitable for printing. No messages appear during the conversion. However if the Ghostview Postscript viewer has been installed and associated with .ps files, then it will be automatically invoked by the GUI. If the viewer does not automatically open, it may be necessary to manually edit the file \quicode\hysplit4.tcl for the directory entry associated with the program gsview32.exe. The sample output from the Postscript file is shown in Fig. 4. The output file can be printed directly on any Postscript printer or printed on any printer through Ghostscript.

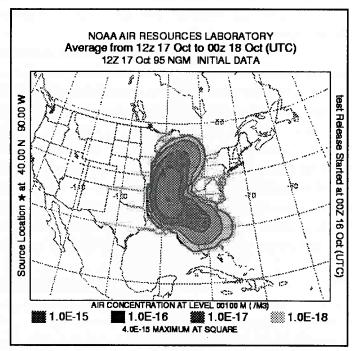


Figure 4. Example from the Postscript conversion.

Step 14 - selecting *Convert to ASCII* will run a program that converts the binary air concentration file to an ASCII file with one record for each grid point giving the latitude-longitude position and air concentration. The file can be used as input to GIS or other visualization programs.

If Tcl/Tk does not exist on your system or there are other problems with the GUI interface, it is very easy to run the sample cases directly in either the \text{trajmdl} or \concmdl sub-directories by double-clicking on hymodelt, wintplot or trajplot for trajectories and hymodelc, wincplot or concplot for air concentrations. If the sample simulation works well, then it is only necessary to manually edit the Control file to try out different simulation variations. The other options are explained in more detail in Section 2.

In general, premature termination during the model initialization phase will result in messages to standard output. However after the model has started, fatal, diagnostic, and progress notification messages are written to a file called *Message*. If the model output is not what you expected, first check the *Control* file to determine if the input setup is what is desired, then check the *Message* file for indication of abnormal performance.

2. ADVANCED SIMULATION CONTROL

When the model starts it looks for an input file called *Control*. If found, this file is used to read all input parameters. If not found, a prompt will appear on standard input requesting appropriate information. These prompts are described in more detail below and are comparable to the appropriate entries through the GUI menu. When data entry is through the keyboard, a file named *Startup* is created. This contains a copy of the input, and later may be renamed to *Control* to permit direct editing and model execution without data entry. If you are unsure as to a value required in an input field, just enter the forward slash (/) character. A default value will be used. This default procedure is valid for all input fields except directory and file names. A automatic default selection procedure is also available when the input fields are read from the *Control* file for certain fields when they are set to zero. Those options are discussed in more detail below. Each input line is numbered (only in this text) according to the order it appears in the file. A number in parenthesis after the line number indicates that there is an input loop and multiple entry lines may be required depending upon the value of the previous entry.

2.1 Trajectories

1- Enter starting time (year, month, day, hour)

Enter the two digit values for the UTC time that the calculation is to start. Use 0's to start at the beginning (or end) of the file according to the direction of the calculation. Zero's will force the calculation to use the time of the first (or last) record of the meteorological data file.

Default: 0000

Default: 1

2- Enter number of starting locations

Simultaneous trajectories can be calculated at multiple levels or starting locations. The maximum number depends upon the compilation parameters. The GUI menu can

accommodate up to 6 simultaneous starting locations. Specification of additional locations requires manual editing of the *Control* file.

3(1)- Enter starting location (lat, lon, m-agl)

Default: 40.0 -90.0 50.0

Position in degrees and decimal (West and South are negative). Height is entered as meters above ground.

4- Enter total run time (hours)

Default: 48

Specify the duration of the calculation in hours. Backward calculations are entered as negative hours.

5- Vertical motion option (0:data 1:isob 2:isen 3:dens 4:sigma)

Default: 0

Indicates the vertical motion calculation method. The default "data" selection will use the meteorological model's vertical velocity fields; other options include isobaric, isentropic, constant density, and constant sigma (internal model coordinate).

6- Top of model domain (internal coordinates m-agl)

Default: 10000.0

Vertical limit of the internal meteorological grid. If calculations are not required above a certain level, fewer meteorological data are processed thus speeding up the computation. Trajectories will terminate when they reach this level.

7- Number of input data grids

Default: 1

Number of simultaneous input meteorological files. The following two entries (directory and name) will be repeated this number of times. Always start with the finest resolution grid as number #1. When the computation shifts from grid #1 to #2, it will not return to #1 again. The run will terminate when the computation is off the last grid. Multiple trajectory calculations will switch grids for all trajectories when the first trajectory passes to the new grid. Multiple grid definitions also have the restriction that there should be some overlap between the grids in space. Time overlap, although desirable, is not required. However, without time overlap it is not possible to interpolate in time across grids hence start trajectories at those times.

8(1)- Meteorological data grid # 1 directory

Default: \main\sub\data\

Directory location of the meteorological file on the grid specified. Always terminate with the appropriate slash (\).

9(2)- Meteorological data grid # 1 file name

Name of the file containing meteorological data. Located in the previous directory.

10- Directory of trajectory output file

Default: \main\trajectory\output\

Directory location to which the ASCII trajectory end-points file will be written. Always terminate with the appropriate slash (\).

11- Name of the trajectory endpoints file

Default: file name

Default: file name

The trajectory end-points output file is named in this entry line. The format of the file is given in Section 6.

2.2 Air Concentration

The entries in the *Control* file for air concentration simulations consist of four groups of input data. The first group is almost identical to the trajectory simulation. The second group defines the pollutant emission characteristics. The third group defines the concentration grid in terms of spacing and integration interval. The fourth group of entries defines pollutant characteristics relevant to computing deposition and removal processes.

2.2.1 Meteorological Simulation Entries

1- Enter starting time (year, month, day, hour)

Default: 0 0 0 0

Enter the two digit values for the UTC time that the calculation is to start. Use 0's to start at the beginning of the file. Note that the calculation start time may be different from the emission start time that is specified below. However the simulation start time may not occur after the emission start time.

2- Number of starting locations

Default: 1

Multiple pollutant sources may be simultaneously tracked. The emission rate specified below is assigned to each source. In addition, the emissions are distributed vertically in a layer between the current emission height and the previous source emission height if the previous source is at the same location. The effective source will be a vertical line source between the two heights. When multiple sources are in different locations, the pollutant is emitted as a point source from each location at the height specified. Point and vertical line sources can be mixed in the same simulation. The GUI menu can accommodate up to 6 simultaneous starting locations. Specification of additional locations requires manual editing of the *Control* file. Area source emissions can be specified from an input file: *emission.txt*. When this file is present in the root directory, the emission parameters in the *Control* file

are superceded by the emission rates specified in the file. More information on this file structure can be found in Section 4.2

3(1)- Enter starting location (lat, lon, m-agl)

Default: 40.0 -90.0 50.0

Position in degrees and decimal (West and South are negative). Height is entered as meters above ground.

4- Enter total run time (hours)

Default: 48

Specify the duration of the calculation in hours. Backward calculations have no meaning in this context.

5- Vertical (0:data 1:isob 2:isen 3:dens 4:sigma)

Default: 0

Indicates the vertical motion calculation method. The default "data" option uses the meteorological model's vertical velocity fields; other options include isobaric, isentropic, constant density, and constant sigma above terrain.

6- Top of model domain (internal coordinates m-agl)

Default: 10000.0

Vertical limit of the internal grid. If calculations are not required above a certain level, fewer meteorological data are processed, thus speeding up the computation. Particles and puffs are restricted from mixing above this level. Complete reflection is assumed.

7- Number of input data grids

Default: 1

Number of simultaneous meteorological fields to be input. The following two entries (directory and name) will be repeated this number of times. Always start with the finest resolution grid as number #1. When the first puff or particle moves on to the next grid, all subsequent particles are automatically transferred to the new grid. There should be time and space overlap for multiple grids.

8(1)- Enter grid # 1 directory

Default: \main\sub\data\

Directory location of the meteorological files. Always terminate with the appropriate (\) slash.

9(2)- Enter grid # 1 file name

Default: file name

Name of the meteorological data file.

2.2.2 Pollutant Definition Entries

10- Number of different pollutants

Default: 1

Multiple pollutant species may be defined for emission. Each pollutant is assigned to its own particle or puff and therefore may behave differently due to deposition or other pollutant specific characteristics. Each will be tracked on its own concentration grid. The following four entries are repeated for each pollutant defined.

11(1)- Pollutant four Character Identification

Default: TEST

Any four-character label that can be used to identify the pollutant. The label is written with the concentration output grid to identify output records associated with that pollutant and will appear in display labels. Additional user supplied deposition and chemistry calculations may be keyed to that identification string.

12(2)- Emission rate (per hour)

Default: 1.0

Mass units released each hour. Units are arbitrary except when specific chemical transformation subroutines are associated with the calculation. Output air concentration units will be in the same units as specified on this line, i.e., input kg/hr -> output kg/m³, input Bq/hr -> output Bq/m³)

13(3)- Hours of emission

Default: 1.0

The duration of emission may be defined in fractional hours. Durations of less than one time-step will be emitted over one time-step, but with the correct total emission requested (rate times duration).

14(4)- Release start time: year month day hour minute Default: [simulation start time]

The previously specified hours of emission start at this time. An entry of zero's in the field, when input is read from a file, will also result in the selection of the default values.

2.2.3 Concentration Grid Definition

Dispersion calculations are performed on the computational (meteorological) grid without regard to the definition or location of any concentration grid. However, the concentration grid spacing may restrict the model's integration time step to a smaller value for higher resolution concentration grids. This section is used to define the grid system to which the concentrations are summed during the integration and subsequently for postprocessing and display of the model's output.

Default: 1

15- Number of simultaneous concentration grids

Multiple or nested grids may be defined. The concentration output grids are treated independently. The following 10 entries will be repeated for each grid defined. The number of grids permitted depends upon model compilation parameters.

16(1)- Center Latitude, Longitude (degrees)

Default: [source location]

The center position of the concentration sampling grid. Input of zero's will result in selection of the default values: location of the emission source.

17(2)- Grid spacing (degrees) Latitude, Longitude

The interval in degrees between nodes of the sampling grid. Puffs must pass over a node to contribute concentration to that point and therefore if the spacing is too wide, they may pass between intersection points. Particle model calculations represent grid-

Default: 1.0 1.0

they may pass between intersection points. Particle model calculations represent gridcell averages, where each cell is centered on a node position, with its dimensions equal to the grid spacing. Finer resolution concentration grids require correspondingly finer integration time-steps. This may be mitigated to some extent by limiting fine resolution grids to only the first few hours of the simulation.

18(3)- Grid span (deg) Latitude, Longitude

Default: [max-Y / d-lat] [max-X / d-lon]

The total span of the grid in each direction. For instance, a span of 10 degrees would cover 5 degrees on each side of the center grid location. A default span is computed from the compiled maximum dimensions of the concentration grid divided by the grid spacing requested in the previous entry.

19(4)- Enter grid # 1 directory

Default: \main\sub\output\

Directory to which the binary gridded concentration output file for this grid is written. As in other directory entries a terminating (\) slash is required.

20(5)- Enter grid # 1 file name

Default: file name

Name of the concentration output file for each grid. See Section 6 for a description of the format of the concentration output file.

21(6)- Number of vertical concentration levels

Default: 1

The number of vertical levels in the concentration grid including the ground surface level if deposition output is required.

22(7)- Height of each level m AGL

Output grid levels may be defined in any order for the puff model as long as the deposition level (0) comes first (a height of zero indicates deposition output). Air concentrations must have a non-zero height defined. A height for the puff model indicates the concentration at that level. A height for the particle model indicates the average concentration between that level and the previous level (or the ground for the first level). Therefore heights for the particle model need to be defined in ascending order.

Default: 50

Default: 0 24 0

23(8)- Sampling start time: year month day hour minute Default: [simulation start time]

Each concentration grid may have a different starting, stopping, and output averaging time. Zero entry will result in setting the default values.

24(9)- Sampling stop time: year month day hour minute Default: {+1} 12 31 24 60

After this time no more concentration records are written. Early termination of high resolution grids (after the plume has moved away from the source) is an effective way of speeding up the computation for high resolution output because that particular grid resolution is no longer used for time-step computations.

25(10)- Sampling interval: type hour minute

Each grid may have its own sampling or averaging interval. The interval can be of two different types: averaging (type=0) or snapshot (type=1). Averaging will produce output averaged over the specified interval. Snapshot will give the instantaneous output at the output interval. For instance you may want to define a concentration grid that produces 24-hour average air concentrations for the duration of the simulation which for the default case of a 2-day simulation will result in 2 output maps, one for each day. Each defined grid can have a different output type and interval.

Default: number of pollutants defined on line # 10

2.2.4 Deposition Definitions

26- Number of pollutants depositing

Deposition parameters must be defined for each pollutant species emitted. Each species may behave differently for deposition calculations. Each will be tracked on its own concentration grid. The following five lines are repeated for each pollutant defined. The number here must be identical to the number on line 10. Deposition is turned off for pollutants by an entry of zero in all fields.

Default: 0.0 0.0 0.0

These three entries are used to define the pollutant as a particle for gravitational settling and wet removal calculations. A value of zero in any field will cause the pollutant to be treated as a gas. All three fields must be defined (>0) for particle deposition calculations. These values need to be correct only if gravitational settling is to be computed by the model, otherwise a nominal value of 1.0 may be assigned as a default for each entry to define the pollutant as a particle. If a dry deposition velocity is specified as the first entry in the next line (28), then that value is used as the particle settling velocity.

28(2)- Deposition velocity (m/s), Pollutant molecular weight (Gram/Mole), Surface Reactivity Ratio. Diffusivity Ratio. Effective Henry's Constant

Default: 0.0 0.0 0.0 0 0.0

Dry deposition calculations are performed in the lowest model layer based upon the relation that the deposition flux equals the velocity times the ground-level air concentration. This calculation is available for gases and particles. The dry deposition velocity can be set directly for each pollutant by entering a non-zero value in the first field or it can be calculated by the model using the resistance method which requires setting the remaining four parameters (molecular weight, surface reactivity, diffusivity, and the effective Henry's constant) - see Table I.

29(3)- Wet Removal: Actual Henry's constant, In-cloud (L/L), Below-cloud (1/s)

Default: 0.0 0.0 0.0

Suggested: 0.0 3.2x10⁵ 5x10⁻⁵

Henry's constant defines the wet removal process for soluble gases. It is defined only as a first-order process by a non-zero value in the field. Wet removal of particles is defined by non-zero values for the in-cloud and below-cloud parameters. In-cloud removal is defined as a ratio of the pollutant in air (g/liter of air in the cloud layer) to that in rain (g/liter) measured at the ground. Below-cloud removal is defined through a removal time constant.

30(4)- Radioactive decay half-life (days)

Default: 0.0

A non-zero value in this field initiates the decay process of both airborne and deposited pollutants.

Table I. Pollutant constants from Wesely (1989)⁴ and Walmsley and Wesely (1996)⁵.

Chemical	Symbol	D _{hx}	H* (M/atm) effective	H(M/atm) actual	f _o
Sulfur dioxide	SO ₂	1.9	1x10 ⁵	1.24	0.0
Ozone	O ₃	1.6	0.01	0.013	1.0
Nitrogen dioxide	NO ₂	1.6	0.01	0.01	0.1
Nitic oxide	NO	1.3	3x10 ⁻³	1.9x10 ⁻³	0.0
Nitric acid	HNO ₃	1.9	1x10 ¹⁴	2.1x10 ⁵	0.0
Hydrogen peroxide	H ₂ O ₂	1.4	1x10 ⁵	1.0x10 ⁵	1.0
Ammonia	NH ₃	0.97	2x10 ¹⁴	62	0.0
Peroxyacetyl nitrate	PAN	2.6	3.6	5	0.1
Nitrous acid	HNO ₂	1.6	1x10 ⁵	2.1x10 ⁵	0

D_{hx} - Diffusivity ratio; H - Henry's constant; f_o - Surface reactivity ratio

31(5)- Pollutant Resuspension (1/m)

Default: 0.0 Suggested: 10⁻⁶

A non-zero value for the resuspension factor causes deposited pollutants to be reemitted based upon soil conditions, wind velocity, and particle type. Pollutant resuspension requires the definition of a deposition grid, as the pollutant is re-emitted from previously deposited material. Under most circumstances, the deposition should be accumulated on the grid for the entire duration of the simulation. Note that the air concentration and deposition grids may be defined at different temporal and spatial scales.

3. GRAPHICAL DISPLAY OPTIONS

The trajectory and concentration models each generate their own output files, which are read by the other programs to produce various displays. The trajectory model generates an ASCII file

⁴Wesely, M.L., 1989, Parameterizations of surface resistances to gaseous dry deposition in regional-scale numerical models, *Atmos. Environ.*, 23, 1293-1304.

⁵Walmsley, J. L., and M.L. Wesely, 1996, Modification of coded parameterizations of surface resistances to gaseous dry deposition, *Atmos. Environ.*, 30, 1181-1188.

of end-point positions while the concentration model produces a binary output file on a regular latitude-longitude grid. All mapping programs use the same ASCII map background file, arlmap, which normally would be located in the \graphics directory. However all the graphics programs search the local start directory first, then the \graphics directory. Customized map background files could be placed in the local directory for specialized applications. Some higher resolution map background files are available from the Hysplit download web page. The Readme.txt file in the \graphics directory has more information about developing custom map background files.

The simple screen display programs and the more feature rich Postscript conversion programs can both be accessed through the GUI or run directly from the command line in a DOS window. The Postscript conversion programs for both trajectories and concentrations have a variety of command line options in which only the default values are available through the GUI. The GUI Postscript conversion defaults can be changed by editing the appropriate lines in the \guicode\hymenu.tcl script.

3.1 Trajectories

The screen display program (wintplot) reads the output file and automatically calculates the most optimum map for display. Multiple starting locations and or heights can be displayed at the same time. Normally the program is invoked directly through the GUI, however the display program can be executed in the \trajmdl directory from the command line:

wintplot [file_name],

where the trajectory endpoint *file_name* is given on the command line. The example output was shown previously in Fig. 1.

The Postscript conversion program (trajplot) also reads the same output file, calculates the most optimum map for display, and creates the output file - trajplot.ps. When executed from the command line, there are three other optional {} inputs:

trajplot [file_name] {Size} {Color} {Labels},

Default: 0 1 12

where Size=0 for standard resolution maps and Size=1 for high resolution maps, Color=0 for black and white output and Color=1 for color differentiation of multiple trajectories, and where Label=0 for no labels along the trajectory, Label=6 for labels every 6 hours, and Label=12 for labels every 12 hours. Default values are shaded. Only the *file_name* is required. The output example was shown previously in Fig. 2.

The format of the ASCII endpoints file written by the trajectory model (*hymodelt*) and read by all display programs is given below:

Record #1

Number of meteorological grids used in calculation

Records Loop #2 through the number of grids

A8 - Meteorological Model identification

- Data file starting Year, Month, Day, Hour, Forecast Hour

Record #3

I6 - number of different trajectories in file

- direction of trajectory calculation (FORWARD, BACKWARD)
- vertical motion calculation method (OMEGA, THETA, ...)

Record 150p #4 through the number of different trajectories in file

4I6 - starting year, month, day, hour 2F8.3 - starting latitude, longitude

F8.3 - starting level above ground (meters)

Record #5

I6 - number (n) of diagnostic output variables

nA8 - label identification of each variable (PRESSURE, THETA, ...)

Record Loon #6 through the number of hours in the simulation

I6 - trajectory number

I6 - meteorological grid number

516 - time of point: year month day hour minute

16 - forecast hour at point

F8.1 - age of the trajectory in hours 2F8.3 - position latitude and longitude

F8.1 - position height in meters above ground

nF8.1 - n diagnostic output variables

3.2 Air Concentration

Concentration graphics can be directed to the screen using wincplot or to a postscript file (concplot.ps) using the concplot program. Wincplot automatically scales the map according to the size of the concentration grid, not the size of the pollutant plume. The map scale can be adjusted by limiting the size of the concentration sub-grid. The size of the grid is specified in the Control file. The display program, wincplot found in the \concmdl directory, is a simplified variation of concplot requiring only the file_name on the command line:

wincplot [file name]

The output example for wincplot was shown previously in Fig. 3.

A concentration output graphic can also be generated using the *concplot* routine, also found in the \concmdl directory, which creates the Postscript output file concplot.ps. Multiple pollutant species or levels can be accommodated. Most routine variations can be invoked from the command line as follows with 6 optional \{\} parameters:

concplot [file_name] {Z1} {Z2} {Type} {Size} {Color} {Value}.

The heights Z1 and Z2 represent the levels that will be displayed. The heights are always defined as meters AGL and should correspond to the range of values defined in the input section (line 22). The level information is interpreted according to the Type definition, such that when:

Type 1, all output levels between the levels specified on the command line are displayed as individual frames. A single level will be displayed if either both specified levels equal the calculation level or they bracket that level. Deposition plots are produced if available in the file and when a level height is set to 0. If level information is omitted, all levels are displayed. When Type=2, the concentrations at all levels between the specified range are averaged to produce one output frame per time period. If a deposition plot is required then Z1 should be set to 0. A customized output is created when Type=3, in that the output concentrations are converted to time-integrated units and vertically averaged for all levels that are found in the file between Z1 to Z2. The last frame displayed represents the accumulated deposition through the model simulation.

The Size specification is set to for standard resolution and "1" for a high resolution map. A high-resolution map has less white space around the concentration pattern. A Color option of "0" will use grey shade patterns for the contour color fill while would use the standard four color fill. The Value parameter is set to "0" if the contour intervals are to be optimized for each map, or set to "1" if they are to be the same for all maps, or set to an integer that represents the power of 10 of the maximum contour. As before, all default values are shown in a shaded highlight.

One final note is that if multiple pollutant species are defined, a prompt to standard output will appear, requesting the selection of a specific species. Only one pollutant species may be displayed per plot sequence. However, an entry of "0" will cause all species to be summed for display.

The output format of the binary concentration file written by *hymodelc* and read by all concentration display programs is as follows:

Record #1

CHAR*4 Meteorological MODEL Identification

INT*4 Meteorological file starting time (YEAR, MONTH, DAY, HOUR, FORECAST)

INT*4 NUMBER of starting locations

Record #2 Loop to record: Number of starting locations

INT*4 Release starting time (YEAR, MONTH, DAY, HOUR)

REAL*4 Starting location and height (LATITUDE, LONGITUDE, METERS)

Record #3

INT*4 Number of (LATITUDE-POINTS, LONGITUDE-POINTS)

REAL*4 Grid spacing (DELTA-LATITUDE, DELTA-LONGITUDE)

REAL*4 Grid lower left corner (LATITUDE, LONGITUDE)

Record #4

INT*4 NUMBER of vertical levels in concentration grid

INT*4 HEIGHT of each level (meters above ground)

Record #5

INT*4 NUMBER of different pollutants in grid CHAR*4 Identification STRING for each pollutant

Record #6 Loop to record: Number of output times

INT*4 Sample start (YEAR MONTH DAY HOUR MINUTE FORECAST)

Record #7 Loop to record: Number of output times

INT*4 Sample stop (YEAR MONTH DAY HOUR MINUTE FORECAST)

Record #8 Loop to record: Number of levels, Number of pollutant types

CHAR*4 Pollutant type identification STRING
INT*4 Output LEVEL (meters) of this record

REAL*4 Concentration output ARRAY (number of lat/lon elements)

There is one additional program, con2asc, that is also part of the GUI interface, which can be used to convert the binary concentration file to a simple ASCII file composed of one record per grid point for all grid points where concentrations at any level are non-zero. Concentrations for multiple levels and pollutant species are all listed on the same record for each grid point. The primary purpose of the conversion is to create a file that can be imported into other applications.

The format of each file record is given by:

213 - End of Sample Julian Day and Hour

F7.2,F8.2 - Latitude and Longitude of grid cell

45E8.2 - Concentration data (by level and pollutant)

A record is identified by the day (Julian: 1 to 365) and hour (UTC) of the ending time of each sample. In addition a new file is created for each sampling period, where the name of the file is composed of the Julian day and hour.

4. SPECIAL APPLICATIONS

This section provides some guidance in configuring the model input to do certain specialized calculations. The default configuration supplied with the test meteorological data is confined to a simple trajectory and inert transport and dispersion calculation. Some other simple configurations will be reviewed in this section.

4.1 Particle or Puff Releases

The concentration model default simulation assumes a particle dispersion in the vertical direction and a top-hat puff dispersion in the horizontal direction. Other options are set with the *INITD* parameter of the *SETUP*. *CFG* namelist file defined in Section 4.4. Normally changes to the dispersion distribution are straightforward. However there are some considerations with regard to the initial number of particles released. The default release is set to be 500 particles over the duration of the emission cycle (see *NUMPAR* in Section 4.4). A 3-dimensional (3D)

particle simulation requires many more particles to simulate the proper pollutant distribution, the number depending upon the maximum downwind distance of the simulation and the duration of the release, longer in each case require more particles. Too few particles result in noisy concentration fields. A 3D puff simulation can be started with one puff as the puff-splitting process in conjunction with the vertical dispersion quickly generates a sufficient number of puffs to represent the complex dispersion process. The default configuration represents a compromise in permitting particle dispersion in the vertical for greater accuracy and puff dispersion in the horizontal to limit the particle number requirements.

4.2 Continuous Emissions

As noted in Section 4.1 the default release is 500 particles over the duration of the emission cycle. If continuous emissions are specified (e.g. over the duration of the simulation), then those 500 particles are spread out over that time period. This may easily result in the release of too few particles each hour to provide smooth temporal changes in the concentration field. Imagine a single particle passing in and out of the vertical concentration grid plane due to turbulent diffusion. One solution would be to increase the *NUMPAR* parameter until smoother results are obtained. Another possibility would be to cycle the emissions by emitting 100 particles only for the first time step of each hour. Those particles would contain the total mass for a one-hour release (see how to set *QCYCLE* as described in Section 4.4).

4.3 Gridded Area Source Emissions

Normally emissions are assumed to be point or vertical line sources. However emissions can also be predefined for a grid. If the model's root startup directory contains the file Emissions.txt, then the pollutants are emitted from each grid cell according to the definitions previously set in the Control file. Two source points should be selected, which define the lower left (1st point) and upper right (2nd point) corner of the emissions grid that will be used in the simulation. This can be a subset of the grid defined in Emissions.txt. The release height represents the height from the ground through which pollutants will be initially distributed. The emission file's first record contains information about the internal grid cell size that is used by the dispersion model to accumulate the file's emissions. The emission file defines the emissions at latititude-longitude points, the values at these points are accumulated in an internal grid, the size of which is defined on the first record. This value can be arbitrarily changed according to the The pollutant puffs are released with an initial size desired resolution of the simulation. comparable to the accumulation cell size. Because the emission file data are remapped to an internal grid, the file can consist of emissions data on a regular grid or just a collection of individual cells. The emission rate in the Control file is used as an additional multiplication factor for the data in the emission file. Also note that previously discussed particle number restrictions still apply. The initial number of particles are spread out over the duration of the emission and the number of grid cells that are defined in the emission domain. The format of the Emission.txt file is given below:

Record #1

I4 - Number (n) of pollutant species in file

F10.4 - Conversion factor from file emission units to internal model units/hour

2F10.4 - Internal grid cell size (latitude & longitude) at which file emissions are accumulated

nA4 - Character identification of each pollutant (should match control file)

Records Loop #2 to the number of i.j grid point

2I4 - I,J grid point index of emission cell (arbitrary units for user identification)

2F10.4 - Southwest corner Longitude and Latitude of this emission cell

Record Loop #3 to the number of pollutant species

12E10.3 - emissions for pollutant#1 hours 1-12 12E10.3 - emissions for pollutant#1 hours 13-24

The model can easily be configured to simulate more complex pollutant episodes with multiple pollutant types or multiple pollutant species on the same particle. This is accomplished by changing either MAXTYP or MAXDIM in DEFSIZE.INC to the appropriate value and recompiling the code. If an external chemistry routine is used that converts mass from one species to another, all tracking together (advecting and dispersing), then MAXDIM is raised to the required value. If multiple species are emitted, have no interaction, and may track differently, then MAXTYP is adjusted to the required value. This latter situation may represent a volcanic ash plume where each pollutant, a different sized particle, settles at a different rate. Note that multiple species defined by the latter method can be accomplished within the default configuration of the model. However the MAXDIM definition always requires an external routine to adjust the mass between species.

4.4 Namelist File: SETUP.CFG

Additional simulation options are available through modification of the Setup.cfg namelist file. This file is not required, and if not present in the root startup directory, default values are used. The trajectory model has only one namelist option. The concentration model has 10 parameters. These parameters can all be changed without recompilation by modification of the contents of Setup.cfg and in some cases their modification will substantially change the nature of the simulation. The file should be present in the root directory (either \working for the GUI interface or \concentral concentral or \tau_indl for command line) with the following contents:

TRATIO - valid for trajectories or concentration simulations and defines the fraction of a grid cell that a trajectory is permitted to transit in one advection time step. Reducing this value will reduce the time step and increase computational times. However, smaller time steps result in less integration error. Integration errors can be estimated by computing a backward trajectory from the forward trajectory end position and computing the ratio of the distance between that endpoint and the original starting point divided by the total forward and backward trajectory distance.

Default value = 0.75

INITD - determines if the model is configured as a puff or particle model. Valid options: 0 (3D particle); 1 (Gaussian Puff); 2 (Top Hat Puff); 3 (Gaussian Particle) 4 (Top-Hat Particle).

Default value = 4

KHMAX - is the maximum age (hours) that any puff or particle is permitted to attain. All pollutants beyond this age are deleted.

Default value = 9999

NUMPAR - would be the maximum number of particles or puffs permitted during a simulation. This value is different from MAXPAR in the include file, in that NUMPAR cannot exceed MAXPAR. NUMPAR has a different meaning for puff and particle simulations. In a full puff simulation, where only one puff per time step is released, the total number of puffs on the grid at any one time cannot exceed NUMPAR. In a particle simulation, or mixed particle-puff simulation, NUMPAR represents the total number of particles that are released during one release cycle. Multiple release cycles cannot produce more than MAXPAR number of particles. For a mixed simulation (particle-puff), NUMPAR should be greater than one but does not need to be anything close to what is required for a full 3D particle simulation.

QCYCLE - are the number of hours between emission cycles. A zero value does nothing. The number of hours of emission specified released. When this value is non-zero, the number of emission hours is repeated again at QCYCLE hours after the starting emission time specified in the input.

Default value = 0.0

KRND - at this interval in hours, enhanced puff merging takes place. Enhanced merging is less restrictive and will degrade the accuracy of the simulation. Puffs can be further apart and still be merged into the same position. Less frequent merging will improve accuracy, however too many puffs may remain and the simulation time will be substantially increased. The selection of an appropriate value depends in part if the pollutant release is instantaneous or continuous.

Default value = 6

FRMR - is the fraction of the mass that is permitted to be removed at KRND intervals. The normal situation is to permit no mass loss. However for certain simulations, such as when a pollutant has a high ambient background relative to the puff concentration, a small removal rate will significantly reduce the number of puffs on the grid at no loss in accuracy.

Default value = 0.0

DELT - can be used to set the integration time step to a fixed value in minutes from 1 to 60 and it should be evenly divisible into 60. The default value of 0.0 causes the program to compute the time step each hour according to the maximum wind speed, meteorological and concentration grid spacing, and the TRATIO parameter. The option to use a fixed time step should only be used when strong winds in regions not relevant to the dispersion simulation are causing the model to run with unrealistically small time steps. Improper specification of the time step could cause aliasing errors in advection as well as substantial underestimates of air concentrations.

Default value = 0.0

ISOT - is a flag used to set the isotropic turbulence option. The default value of 0 results in the computation of vertical turbulence from vertical stability estimates and the horizontal turbulence from the wind field deformation. In shorter range dispersion simulations (<100 km) the deformation parameterization used in conjunction with larger scale meteorological fields will not reflect the diurnal variations in horizontal turbulence. In these situations isotropy is assumed by setting the ISOT parameter to 1, i.e., the horizontal velocity variance is set equal to the vertical velocity variance. In addition, the vertical diffusivity profile is NOT replaced by its boundary layer average value when ISOT=1.

NDUMP - can be set to dump out all the particle/puff points at the end of a simulation to a file called PARDUMP. This file can be read from the root directory at the start of a new simulation to continue the previous calculation. Valid NDUMP settings: 0 - no I/O, 1- read and write, 2 - read only, 3 - write only.

Default value = 0

4.5 Compilation Limits: DEFSIZE.INC

A variety of different parameters are set in the compilation "include" files. The value of some of these parameters may effect the results of a simulation and the options that are available in setting up the *Control* file. There is a copy of the *DEFSIZE.INC* include file in each subdirectory: trajectories, air concentrations, and other special applications. The parameters in the local include file are optimized for the application in that directory. A summary of the main features of the primary "include" file *DEFSIZE.INC* follows:

Meteorological grid size parameters ...

NXYD - The product of the number of points in X and Y of the packed meteorological data grid should not exceed this value.

NXM, NYM - The horizontal limits of the meteorological sub-grid. Note this value may be larger or smaller than the actual data grid on the input file. It only specifies how much data is read and processed from the input file at any one time. This is the prime dimension controlling memory requirements because all meteorological variables are of this dimension. These values are usually kept small for trajectory calculations; you do not need to process the whole grid to compute advection at only one point. However for concentration simulations, it is best if a larger grid domain can be loaded, because pollutant plumes usually encompass a much larger area. A small sub-grid for concentration simulations may cause the model to keep reloading the data at the same time but slightly different locations to complete a calculation.

NZM - In a similar manner to the horizontal dimension, it limits the scope of the model's internal coordinate system in that only meteorological data from the ground to NZM number of levels are processed. In addition, the internal vertical grid to which the meteorological data are intepolated is of the same dimension.

MLVL, MVAR - define the maximum data levels and parameters that may be found on an input file. It is necessary that these parameters cover the scope of potential input files as the model must be able to read the index record of the data file. This record will contain information for each level and variable.

MGRD - permits the simultaneous definition of multiple meteorological input files. The ability to open multiple files has low memory requirements. However multiple files may slow calculations as only one file's data are permitted in memory at any one time.

Additional parameters for concentration calculations...

MAXPAR - is the maximum number of particles or puffs that may be followed for the compiled version of the code. Larger values require correspondingly more system memory. The actual particle/puff limit during a particular calculation is set in the namelist file.

MAXDIM - The maximum number of different species that can be associated with any single particle or puff. There is no routine model configuration that requires this value to be greater than one. Certain optional additional subroutines may be added that may convert mass from one species to another on the same particle or puff.

MAXTYP - The number of different pollutant species. Each species is associated with a different puff or particle. MAXTYP should always be equal to or greater than MAXDIM. Different pollutant types may be defined as part of the normal input procedure for emissions and deposition.

MAXGRD - The number of simultaneous concentration output grids. Values larger than one quickly increase memory requirements because each grid will have the dimensions: MAXXP, MAXYP, MAXTYP, MAXTYP, MAXGRD.

MAXXP, MAXYP - The maximum number of points in the West to East direction and the South to North direction on any concentration grid.

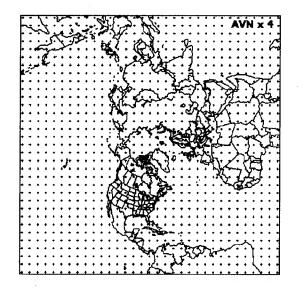
MAXZP - The maximum number of levels on any concentration grid.

To increase the number of sources for trajectories and concentrations ...

MLOC - the number of simultaneous trajectories or particle starting locations that can be simultaneously tracked during a computation.

5. METEOROLOGICAL INPUT DATA

Meteorological data fields to run the model are usually already available from routine archives or from forecast model outputs. Archive meteorological data to run the model may be ordered from NOAA's National Climatic Data Center⁶ or more recent data files can be copied from ftp://gus.arlhq.ssmc.noaa.gov/pub/archives. There are more complete descriptions of the different data sets available on-line. Figs. 5 and 6 illustrate the domain of the global Aviation model data, applicable to both archives and forecasts, available at a 181 km resolution but shown only at every fourth grid point.



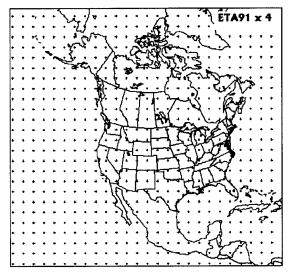
AVN x 4

Figure 5. Global northern hemisphere grid.

Figure 6. Global southern hemisphere grid.

Note that the NCEP models are run at much higher spatial resolution than what is archived in a Hysplit compatible format. If calculations at higher resolution are required, then the original GRIB encoded files must be obtained and converted as described later in this section. Although sample software is provided, no additional guidance except for the information contained in this report is available. Higher resolution data over North America using the ETA model forecasts on a 91 km grid is shown in Fig. 7. The ETA data analysis and assimilation (EDAS) archive grid at 80 km resolution is shown in Fig. 8. Both illustrations only show every fourth grid point for clarity.

⁶Climate Services Branch, National Climatic Data Center, 151 Patton Avenue, Asheville, NC 28801, http://www.ncdc.noaa.gov, archives: TD-6140 and TD-6141.



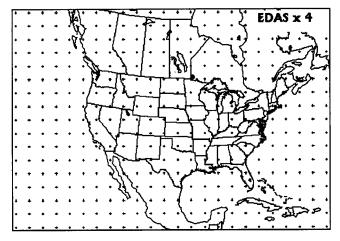


Figure 7. ETA forecast model grid.

Figure 8. EDAS archive data grid.

The following sections describe the data in a little more detail so that customized applications can be developed. Additional subroutines are provided to simplify the task of creating a model compatible data file. This data file is composed of one or more time periods of data. Each time period begins with one or more ASCII index records that summarize the time period, the grid definition, variable and level information. Each subsequent record contains one horizontal data field, consisting of 50 ASCII bytes of time, variable, and level information for that record, followed by X times Y bytes of data, where X and Y are the number of data points in each direction. Floating point or integer data are packed as one byte per variable. Precision is maintained by packing the differences between adjacent grid points rather than packing the absolute values. In any one time period, although not required, the surface data precede the upper-level data fields. All records are the same length because the model needs to read the file in "direct access" mode. Data files can be read on most computing platforms without any transformation and appended to each other using routine operating system commands. Only binary transfers or copies are permitted. All of the routines discussed in this section can be found in the \methatalsource directory.

5.1 Valid Meteorological Data Types

Meteorological variables are identified to the model by a unique 4 character identification that is written to the first 50 byte header portion of each data record. Some of the variables that can be decoded by the model and their units are identified below.

Surface-Level Parameters Description	<u>Units</u>	<u>Identification</u>
Pressure at surface	hPa	PRSS
Pressure reduced to mean sea level	hPa	MSLP
Temperature at surface	K	TMPS
Total precipitation (6-h accumulation)	m	TPP6
Momentum flux, u-component at surface	N/m^2	UMOF

Momentum flux, v-component at surface	N/m^2	VMOF
Sensible heat net flux at surface	W/m^2	SHTF
Latent heat net flux at surface	W/m^2	LHTF
Sfc downward short wave radiation flux	W/m^2	DSWF
Temperature at 2 m AGL	K	T02M
Relative humidity at 2 m AGL	%	RH2M
U-component of wind at 10 m AGL	m/s	U10M
V-component of wind at 10 m AGL	m/s	V10M
Volumetric soil moisture content (<10cm)	fraction	SOLW
Total cloud cover, entire atmosphere	%	TCLD
Town troub to vor, ontire atmosphere	,,,	1422
Upper-level Parameters Description	<u>Units</u>	Identification
•		
Upper-level Parameters Description	Units	Identification
Upper-level Parameters Description U-component of wind with respect to grid	<u>Units</u> m/s	Identification UWND
Upper-level Parameters Description U-component of wind with respect to grid V-component of wind with respect to grid	<u>Units</u> m/s m/s	Identification UWND VWND
Upper-level Parameters Description U-component of wind with respect to grid V-component of wind with respect to grid Geopotential height	Units m/s m/s gpm*	Identification UWND VWND HGTS

Data may be obtained from any source, however there are certain minimum data requirements to run the model: surface pressure or terrain height, u-v wind components, temperature, and moisture. In addition, precipitation is required for wet removal calculations. Not required, but certainly necessary to improve vertical mixing calculations would be some measure of low-level stability. This may take the form of a near-surface wind and temperature or the fluxes of heat and momentum.

It is also important to have sufficient vertical resolution in the meteorological data files. Some of the NOAA higher resolution data files have five or more levels in the boundary layer (<850 hPa) in addition to wind and temperatures near the surface, usually 2 and 10 m agl. These surface values are especially important when the data are only available on absolute pressure surfaces, rather than terrain following sigma surfaces, to avoid interpolation to the surface between data levels when the local terrain is well above sea-level.

5.2 Creation of a Meteorological Input Data File

One may prepare data from other sources to be in a suitable format for the model through a series of routines described in this section. In general it is assumed you have access to some meteorological data source, either the data fields are already on a grid, such as output from a meteorological model, or perhaps observations that have been interpolated to a grid. Some example conversion programs are provided to convert from either NOAA, NCAR (re-analysis), or ECMWF GRIB format data files to Hysplit format (see avn2arl, ncr2arl, ecm2arl in directory ldata2arl). If these programs are to be used directly, it will be necessary to obtain special platform dependent GRIB decoding subroutines. These are usually provided in conjunction with the GRIB data.

The meteorological data are processed in time-sequence, calling the subroutines provided, to create a Hysplit compatible output file. These subroutines will pack the data and write the

index record. The index record, which precedes the data records for each time period, can only be written after the data records are processed. The routine must first be initialized by setting all the appropriate grid parameters and defining the meteorological variables that will be written to the file. Multiple output grids may be defined and written simultaneously by invoking the *PAKSET* routine with a different unit number for each grid. The grid parameters are all defined in a configuration file which should be in the directory from which the procedure is invoked:

CALL PAKSET(kunit, fname, krec, nx, ny, nz).

Kunit is the Fortran unit number to which the data records will be written. Fname is the character string of the name of the configuration file. It can be any name, but it will default to metdata.cfg. The file is opened internally on kunit to read the configuration file. This routine needs to be called once for each grid. Krec is the starting record number (of the index record) to which output will be written. It is normally set to 1 unless you are writing to the middle of a file. The remaining parameters (nx, ny, nz) are returned by the subroutine and define the horizontal and vertical grid dimensions. These values can be used to set variable dimensions. It is your responsibility to open kunit for output after having completed the pakset calls:

```
OPEN(file = , unit = kunit, form = 'unformatted', access = 'direct', recl = \{50 + nx*ny\})
```

The individual data records are packed and written by a call to *PAKREC*, once for each variable at each level. The routine calculates the record offset from the index record according to the variable and level information provided in the arguments and writes the record according to the order specified in *metdata.cfg*. The data can be supplied in any order. Note that although the level indicator (*ll*) goes from 1 to the number of levels, one is subtracted before it is written to the 50 byte header to be consistent with the definition of surface data to be at level "0". All the records in a time period may be initialized according to the value of the *kimi* flag. Initialization fills in the time variable for all records and assigns the variable identification field as *null*.

CALL PAKREC(kunit,rvar,cvar,nx,ny,nxy,kvar,iy,im,id,ih,mn,ic,ll,kini)

```
- integer unit number of the defined file
kunit
              - input array of real*4 data values
rvar
              - character*1 array of packed data values
cvar
              - integer horizontal grid dimensions
nx,ny
              - integer product nx*ny and length of cvar
nxy
              - character*4 descriptor of variable being written
kvar
iy,im,id,ih
             - integer time identification
              - integer minutes associated with the time (usually 0)
mn
              - integer forecast hour (hours from initialization)
ic
11
              - integer level indicator (1 to NZ)
              - integer time period initialization flag (0-no; 1-yes)
kini
```

When all the data records for a time period have been written, it is necessary to close that time period by writing its index record:

CALL PAKNDX(kunit).

At this point your program can return to *PAKREC* if data records for additional time periods are to be added to the file.

The key to the process is creating the proper configuration file for the data set you want to create. A sample *metdata.cfg* file for NOAA's NGM is shown below. The format is such that the first 20 characters are a dummy identification field followed by the data.

20X.Format	Column_1 ID	Column_21 DATA
A4	Data Source:	NGM
I4	Grid Number:	6
I 4	Z-Coordinate:	1
F10	Pole Latitude:	90.0
•••	Pole Longitude:	0.0
•••	Reference Latitude:	60.0
•••	Reference Longitude:	-105.0
•••	Reference grid size:	182.9
•••	Orientation:	0.0
•••	Tangent Latitude:	90.0
•••	Synch point X:	13.25
•••	Synch point Y:	42.75
•••	Synch Latitude:	90.0
•••	Synch Longitude:	0.0
•••	Reserved:	0.0
I 4	Number X points:	33
I4	Number Y points:	28
I 4	Number of Levels:	11
F6.,I3,(1X,A4)	Level 1:	1.0000 04 TPPT EXCO HFLX PRSS
•••	Level 2:	0.9823 05 UWND VWND WWND SPHU TEMP
•••	Level 3:	0.9432 05 UWND VWND WWND SPHU TEMP
•••	Level 4:	0.8967 05 UWND VWND WWND SPHU TEMP
•••	Level 5:	0.8437 05 UWND VWND WWND SPHU TEMP
•••	Level 6:	0.7848 05 UWND VWND WWND SPHU TEMP
•••	Level 7:	0.7210 05 UWND VWND WWND SPHU TEMP
•••	Level 8:	0.6531 05 UWND VWND WWND SPHU TEMP
•••	Level 9:	0.5820 05 UWND VWND WWND SPHU TEMP
•••	Level 10:	0.5086 05 UWND VWND WWND SPHU TEMP
•••	Level 11:	0.4341 05 UWND VWND WWND SPHU TEMP

It is important that the information contained in this file is correct as it not only controls the writing of the file, but much of the information is written into the index record of each time period. The model decodes this information to set up the internal processing of the meteorological data. A complete description of *metdata.cfg* follows:

Record 1 consists of a four character string that identifies the source of the meteorological data. This string will be passed through to many of the output graphics.

Record 2 is an optional integer identification of the meteorological data grid. It was used extensively in previous meteorological data file formats. It is not used in Hysplit_4 applications.

Record 3 is an integer number that identifies the vertical coordinate system. Only four coordinate types are recognized: 1-pressure sigma; 2-pressure absolute; 3-terrain sigma; 4-hybrid sigma.

Records 4 & 5 identifies the pole position of the grid projection. Most projections will either be defined at +90 or -90 depending upon the hemisphere. The longitude would be the point 180 degrees from which the projection is cut.

Records 6 & 7 is the reference position at which the grid spacing is defined.

Record 8 is the grid spacing in km at the reference position.

Record 9 is the grid orientation or the longitude of the meridian which is parallel to the up-down direction of the grid.

Record 10 is the angle between the axis and the surface of the cone. For regular projections it is equal to the latitude at which the grid is tangent to the earth's surface. A polar stereographic grid would be tangent at either 90 or -90, while a Mercator projection is tangent at 0 latitude. A Lambert Conformal projection would be in between the two limits. An oblique stereographic projection would have a cone angle of 90.

Records 11 & 12 are used to equate a position on the grid with a position on the earth as given in Records 13 & 14. In this example, the position indicated is the center of the grid located over the North Pole. Any position is acceptable. It need not even be on the grid.

Record 15 is not currently used.

Records 16 & 17 identify the number of grid points in each direction.

Record 18 is the number of levels in the vertical, including the surface level.

Record 19, through the number of levels, identifies the height of each level in appropriate units according the definition of the vertical coordinate, the number of variables at that level, and the four character identification string for each variable. The height units are as follows for each coordinate: 1-sigma (fraction); 2-pressure (mb); 3-terrain (fraction); 4-hybrid (mb-offset.fraction)

5.3 Decoding Meteorological Data Files

One may want to develop other applications for Hysplit compatible meteorological data files. For these situations, some lower-level routines are provided in the source code library. The key to reading the meteorological files is decoding the index record. The format for this record is given below. Complete descriptions are similar to the variables in the discussion above.

FORMAT	DESCRIPTION
A4	Data Source
I3	Forecast hour (>99 the header forecast hr = 99)
12	Minutes associated with data time

12F7.	1) Pole Lat, 2) Pole Long, 3) Tangent Lat, 4) Tangent Long, 5) Grid Size, 6)Orientation, 7) Cone Angle, 8) X-Synch point, 9) Y-Synch point, 10) Synch point lat, 11) Synch point long, 12) Reserved
3I3	1) Number x points, 2) Number y points, 3) Number levels
I2	Vertical coordinate system flag
I4	Length in bytes of the index record, excluding the first 50 bytes

LOOP through the number of data levels

F6.	height	of the first level

I2 number of variables at that level

LOOP through the number of variables

A4	variable identification
A4	variable identification

I3 rotating checksum of the packed data

1X Reserved space for future use

Once the index record has been read and decoded you have sufficient information to read and decode the data records. An un-packer is provided to convert the packed character*1 array to a real*4 array. It can also be used to extract a sub-grid from the full domain through specification of the sub-grid lower left corner:

CALL PAKINP(rvar,cvar,nx,ny,nx0,ny0,lx,ly,prec,nexp,var1,ksum)

```
rvar - real output array of integer dimensions lx,ly cvar - character*1 packed input array of length nx*ny
```

nx,ny - integer dimensions of the full grid

nx0 - integer sub-grid position of left edge in nx units
 ny0 - integer sub-grid position of lower edge in ny units

lx - integer first dimension of sub-grid length
 ly - integer second dimension of sub-grid length

prec - real precision of packed data array

nexp - integer scaling exponent of packed data array

var1 - real value of array at position (1,1)

ksum - integer rotating checksum of packed data array

If the entire grid is to be unpacked then nx0=ny0=1 and nx=lx, ny=ly. The checksum (ksum) that is returned should be compared with the corresponding value in a table generated from reading the index record. If you are not going to compare the checksum, set ksum = -1, this will save a little computer time. Due to the sub-grid option the checksum cannot be computed in the regular unpacking loop, but requires a second pass through the data. The checksum pass is enabled when ksum=0. It will then return a non-zero value. If you don't reset it to zero, no further checksums will be computed.

If you want to create your own packed data by converting a real*4 array to the character*1 packed data array use the following:

CALL PAKOUT(rvar,cvar,nx,ny,nxy,prec,nexp,var1,ksum)

Although the structure of the packed data may seem complex, unpacking is a very simple process, the basic elements of which are summarized in the Fortran code shown below. The value of each element is the sum of the initial value and the difference stored in that element location.

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

CHARACTER*1 CPACK (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 (CPACK (INDX)) -127.) / SCALE+VOLD

VOLD=RVAR (I, J)

END DO

VOLD=RVAR (I, J)

END DO

RETURN
```

5.4 Sample Meteorological Programs

The source code for many different meteorological data applications can be found in /metdata and /data2arl. Most of these programs require the routines found in /metdata/source. In addition, utility programs that convert GRIB formatted meteorological data files require GRIB decoding routines specific to the meteorological center that created the GRIB files; ECMWF decoders are provided with the data, NOAA decoders are available from the NCEP web site. In addition many of the GRIB decoders use some platform specific subroutines to read variable length records in Fortran in a direct-access mode. This customized software is not provided, but can be replicated through slower conventional Fortran methods.

Programs found in \metdata:

chk_rec - program to dump the first 50 bytes of each meteorological data record. Those bytes contain ASCII data describing the packing.

chk_file - program to examine header and data records of an ARL packed meteorological data file. The program uses the same I/O subroutines common to Hysplit code. If this program does not work with your data file, neither will Hysplit.

profile - creates text file of the profile of meteorological variables at a specified location and time. The output written to the screen and to the file - profile.txt.

display - creates postscript file of meteorological data contoured and color filled for a single variable at a specified time. Output written to display.ps

Programs found in \data2arl:

rsm2arl - decodes the Regional Spectral Model (RSM) GRIB output fields on sigma surfaces to ARL packed format.

prsm2arl - decodes the Regional Spectral Model (RSM) GRIB output fields on pressure surfaces to ARL packed format.

avn2arl - decodes NOAA Aviation model GRIB fields and converts them to ARL packed format.

ncr2arl - decodes NCEP/NCAR re-analysis GRIB fields and converts them to ARL packed format.

ecm2arl - decodes ECMWF model GRIB fields and converts them to ARL packed format. Requires ECMWF supplied GRIBEX subroutines.

dat2arl - creates a packed meteorological file for Hysplit using dummy fields hardwired into the program. The input meteorological data subroutines should be replaced by routines reading user supplied meteorological data files.

content - decodes NOAA grib sections without using the W3LIB routines. This program does not unpack the data but only lists the contents of the GRIB file.

inventory - decodes all the records within a NOAA grib file (without unpacking) providing content information. The program does not use the W3LIB libraries.

unpacker - decodes NOAA grib sections to a real data array without using the W3LIB routines.

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